

STIC Search Report Biotech-Chem Library

STIC Database Tracking Number: 151078

TO: Susan Hanley

Location: rem/3d70/3e71

Art Unit: 1651

Tuesday, April 26, 2005

Case Serial Number: 10/047251

From: Barb O'Bryen

Location: Biotech-Chem Library

Remsen 1a69

Phone: 571-272-2518

BOB

barbara.obryen@uspto.gov

Search Notes	
	·



10/047,251

Text search request:

1 1-1

Is there any report of a compound being administered to a plant or plant cell culture in order to accomplish any of the following process:

- a. Does the compound inhibit any extracellular (or extra-cellular) phosphatase in a plant?
- b. Does the compound decrease drug resistance in plants?
- c. Does the compound inhibit (down-regulate, antagonist, etc) an ABC transporter (also known as an ABC-binding cassette) in a plant cell?

All I need are the Bib Abs, no compound structures.

Thanks. Please call me if you have any questions. 2-2508

Susan

CI COM

LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, HODOC*, RTECS*, TOXCENTER, USPATFULL (*File contains numerically searchable property data)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

170 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

170 REFERENCES IN FILE CAPLUS (1907 TO DATE)

10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'HOME' ENTERED AT 17:12:44 ON 25 APR 2005

=>

VAR G1=1/28
REP G2=(1-5) CH2
VAR G3=O/S
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 40
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 41

STEREO ATTRIBUTES: NONE

L15 312262 SEA FILE=REGISTRY ABB=ON (2 333.151/RID) OR (591.146/RID OR

591.261/RID)

L18 816 SEA FILE=REGISTRY SUB=L15 SSS FUL L3

(FILE 'HOME' ENTERED AT 16:37:16 ON 25 APR 2005)

FILE 'REGISTRY' ENTERED AT 16:37:31 ON 25 APR 2005

L1 STR

L2 0 SEA SSS SAM L1

L3 STR L1

L4 0 SEA SSS SAM L3

FILE 'LREGISTRY' ENTERED AT 16:42:15 ON 25 APR 2005

L5 STR L1

L6 38 SEA SSS SAM L5

D STR RSD

D STR RSD 20

L7 STR

L8 44 SEA SSS SAM L7

```
D STR RSD
                 D STR RSD 10
                 D STR RSD 20
                 D STR RSD 30
 L9
              42 SEA ABB=ON C5S-C6/EA
               O SEA ABB=ON L8 AND L9
 L10
                 STR L7
 L11
 L12
               0 SEA SSS SAM L11
               7 SEA SSS FUL L11
 L13
                 D STR RSD 1-3
      FILE 'REGISTRY' ENTERED AT 16:46:34 ON 25 APR 2005
                 E 333.151/RID
                 E 591.146/RID
                 E 591.261/RID
      FILE 'LREGISTRY' ENTERED AT 16:47:07 ON 25 APR 2005
              89 SEA ABB=ON 2 333.151/RID
 L14
      FILE 'REGISTRY' ENTERED AT 16:47:27 ON 25 APR 2005
 L15
          312262 SEA ABB=ON (2 333.151/RID) OR (591.146/RID OR 591.261/RID)
                 D OUE L3
               O SEA SUB=L15 SSS SAM L3
L16
· L17
               O SEA SUB=L15 SSS SAM L3
 L18
             816 SEA SUB=L15 SSS FUL L3
                 SAVE TEMP L18 HAN251FULL/A
 L19
                 ANALYZE L18 1- LC:
                                          21 TERMS
                 D 1-21
      FILE 'ZCAPLUS' ENTERED AT 16:51:43 ON 25 APR 2005
                 E PLANTS+ALL/CT
      FILE 'REGISTRY' ENTERED AT 16:52:09 ON 25 APR 2005
 L20
               1 SEA ABB=ON PHOSPHATASE/CN
      FILE 'STNGUIDE' ENTERED AT 16:52:16 ON 25 APR 2005
      FILE 'CAPLUS' ENTERED AT 16:56:59 ON 25 APR 2005
 L21
             555 SEA ABB=ON L18
 L22
           14285 SEA ABB=ON L20
 L23
            3894 SEA ABB=ON HERBICIDE RESISTANCE/CT
 L24
           25952 SEA ABB=ON DRUG RESISTANCE/CT
 L*** DEL
               0 S DRUG#(L)SUSEPTIB?
 L25
            7729 SEA ABB=ON PLANT CELL/CT
 L26
           53514 SEA ABB=ON
                             PLANT#/CT OR EMBRYOPHYTA/CT
 L27
          321071 SEA ABB=ON PEA#/OBI OR CARROT#/OBI OR RICE/OBI OR WHEAT/OBI
                 OR CORN/OBI OR SOYBEAN#/OBI OR SOY BEAN#/OBI
 L28
           75717 SEA ABB=ON ZEA MAYS/OBI OR MAIZE/OBI OR GLYCINE MAX/OBI OR
                 TRITICUM/OBI OR ORYZA SATIVA/OBI OR DAUCUS CAROTA/OBI OR PISUM
                 SATIVUM/OBI
 L29
           31428 SEA ABB=ON CROP#/OBI
 L30
            1084 SEA ABB=ON ABC/OBI(W) (TRANSPORTER#/OBI OR BINDING CASSETTE#/OB
                 I)
 L31
            2879 SEA ABB=ON ATP BINDING CASSETTE#/OBI
                 E SUSCEPT
 L32
            2483 SEA ABB=ON DRUG#/OBI(L)SUSCEPTIB?/OBI
 L33
               9 SEA ABB=ON L21 AND (L22 OR L23 OR L24 OR L25 OR L26 OR L27 OR
                 L28 OR L29 OR L30 OR L31 OR L32)
                 D SCAN
 L34
               4 SEA ABB=ON L21(L)AGR/RL
```

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L35
             11 SEA ABB=ON
                            5/SC, SX AND L21
                E 15A/SC
L36
          23905 SEA ABB=ON
                            15A/SC,SX
L37
              3 SEA ABB=ON
                           L21 AND L36
     FILE 'STNGUIDE' ENTERED AT 17:03:03 ON 25 APR 2005
     FILE 'USPATFULL' ENTERED AT 17:04:49 ON 25 APR 2005
L38
             80 SEA ABB=ON L18
L39
            564 SEA ABB=ON
                           L20
L40
            834 SEA ABB=ON HERBICIDE RESISTANCE/CT
L41
           1064 SEA ABB=ON
                           DRUG RESISTANCE/CT
L42
           2528 SEA ABB=ON
                            PLANT CELL/CT
L43
           3334 SEA ABB=ON PLANT#/CT OR EMBRYOPHYTA/CT
L44
          13658 SEA ABB=ON (PEA# OR CARROT# OR RICE OR WHEAT OR CORN OR
                SOYBEAN# OR SOY BEAN#)/IT
L*** DEL
          55243 S CROP#
L45
             89 SEA ABB=ON
                            (ABC(W)(TRANSPORTER# OR BINDING CASSETTE#))/IT, TI, A
                B, CLM
L46
            214 SEA ABB=ON (ATP BINDING CASSETTE#)/IT, TI, AB, CLM
            249 SEA ABB=ON (DRUG#(L)SUSCEPTIB?)/IT
T.47
L48
            652 SEA ABB=ON CROP#/IT
           4659 SEA ABB=ON (ZEA MAYS OR MAIZE OR GLYCINE MAX OR TRITICUM OR
L49
                ORYZA SATIVA OR DAUCUS CAROTA OR PISUM SATIVUM)/IT
L50
              4 SEA ABB=ON L38 AND (L39 OR L40 OR L41 OR L42 OR L43 OR L44 OR
                L45 OR L46 OR L47 OR L48 OR L49)
     FILE 'STNGUIDE' ENTERED AT 17:06:12 ON 25 APR 2005
     FILE 'BIOSIS, TOXCENTER' ENTERED AT 17:08:50 ON 25 APR 2005
L51
             60 SEA ABB=ON L18
L52
          20754 SEA ABB=ON L20
L53
         167544 SEA ABB=ON PHOSPHATASE#
L54
           1357 SEA ABB=ON APYRASE#
L55
         121731 SEA ABB=ON (SUSCEPTIB? OR RESIST?) (5A) (DRUG# OR MULTIDRUG# OR
                HERBICID? OR PESTICID?)
L56
       2820856 SEA ABB=ON PLANT#
L57
         286201 SEA ABB=ON CROP#
L58
         679166 SEA ABB=ON PEA# OR CARROT# OR RICE OR WHEAT OR CORN OR
                SOYBEAN# OR SOY BEAN#
L59
           2947 SEA ABB=ON ABC(W) (TRANSPORTER# OR BINDING CASSETTE#)
L60
           4891 SEA ABB=ON (ATP BINDING CASSETTE#)
L61
         171387 SEA ABB=ON (ZEA MAYS OR MAIZE OR GLYCINE MAX OR TRITICUM OR
                ORYZA SATIVA OR DAUCUS CAROTA OR PISUM SATIVUM)
L62
              8 SEA ABB=ON L51 AND (L52 OR L53 OR L54 OR L55 OR L56 OR L57 OR
                L58 OR L59 OR L60 OR L61)
     FILE 'REGISTRY' ENTERED AT 17:10:28 ON 25 APR 2005
                D STAT QUE L18
     FILE 'CAPLUS' ENTERED AT 17:10:42 ON 25 APR 2005
                D QUE NOS L33
                D QUE NOS L34
                D QUE NOS L35
                D QUE NOS L37
             17 SEA ABB=ON L33 OR L34 OR L35 OR L37
L63
     FILE 'USPATFULL' ENTERED AT 17:11:08 ON 25 APR 2005
```

D QUE NOS L50

FILE 'BIOSIS, TOXCENTER' ENTERED AT 17:11:08 ON 25 APR 2005 D QUE NOS L62

FILE 'CAPLUS, USPATFULL, BIOSIS, TOXCENTER' ENTERED AT 17:11:18 ON 25 APR 2005

L64

23 DUP REM L63 L50 L62 (6 DUPLICATES REMOVED) ANSWERS '1-17' FROM FILE CAPLUS ANSWERS '18-19' FROM FILE USPATFULL ANSWERS '20-22' FROM FILE BIOSIS ANSWER '23' FROM FILE TOXCENTER D IBIB ED ABS HITSTR 1-19

D IALL 20-23

FILE 'STNGUIDE' ENTERED AT 17:11:50 ON 25 APR 2005

FILE 'REGISTRY' ENTERED AT 17:12:36 ON 25 APR 2005 L65 2 SEA ABB=ON 1846-76-0 OR 51081-69-7 D IDE 1-2

FILE 'HOME' ENTERED AT 17:12:44 ON 25 APR 2005 D SAVED D QUE L18

. FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 APR 2005 HIGHEST RN 849094-71-9 DICTIONARY FILE UPDATES: 24 APR 2005 HIGHEST RN 849094-71-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

* The CA roles and document type information have been removed from * * the IDE default display format and the ED field has been added, effective March 20, 2005. A new display format, IDERL, is now available and contains the CA role and document type information. ******************

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

FILE LREGISTRY LREGISTRY IS A STATIC LEARNING FILE

NEW CAS INFORMATION USE POLICIES, ENTER HELP USAGETERMS FOR DETAILS.

Searched by Barb O'Bryen, STIC 2-2518

FILE ZCAPLUS

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FILE COVERS 1907 - 25 Apr 2005 VOL 142 ISS 18 FILE LAST UPDATED: 24 Apr 2005 (20050424/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Apr 22, 2005 (20050422/UP).

FILE CAPLUS

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FILE USPATFULL

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 21 Apr 2005 (20050421/PD) FILE LAST UPDATED: 21 Apr 2005 (20050421/ED)

HIGHEST GRANTED PATENT NUMBER: US6883176

HIGHEST APPLICATION PUBLICATION NUMBER: US2005086720

CA INDEXING IS CURRENT THROUGH 21 Apr 2005 (20050421/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 21 Apr 2005 (20050421/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2005

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2005

>>> USPAT2 is now available. USPATFULL contains full text of the <>< original, i.e., the earliest published granted patents or <>< applications. USPAT2 contains full text of the latest US <>> publications, starting in 2001, for the inventions covered in <>> USPATFULL. A USPATFULL record contains not only the original <><

>>>	published document but also a list of any subsequent	<<'<
>>>	publications. The publication number, patent kind code, and	<<<
>>>	publication date for all the US publications for an invention	<<<
>>>	are displayed in the PI (Patent Information) field of USPATFULL	<<<
>>>	records and may be searched in standard search fields, e.g., /PN,	<<<
>>>	/PK, etc.	<<<
>>>	USPATFULL and USPAT2 can be accessed and searched together	<<<
>>>	through the new cluster USPATALL. Type FILE USPATALL to	<<<
>>>	enter this cluster.	<<<
>>>		<<<
>>>	Use USPATALL when searching terms such as patent assignees,	<<<
>>>	classifications, or claims, that may potentially change from	<<<
>>>	the earliest to the latest publication.	<<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BIOSIS FILE COVERS 1969 TO DATE. CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 20 April 2005 (20050420/ED)

FILE RELOADED: 19 October 2003.

FILE TOXCENTER

=>

FILE COVERS 1907 TO 19 Apr 2005 (20050419/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TOXCENTER has been enhanced with new files segments and search fields. See HELP CONTENT for more information.

TOXCENTER thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2005 vocabulary. See http://www.nlm.nih.gov/mesh/ and http://www.nlm.nih.gov/pubs/techbull/nd04/nd04_mesh.html for a description of changes.

STIC-Biotech/ChemLib

From:

Chan, Christina

Sent:

Monday, April 25, 2005 2:30 PM

To:

Hanley, Susan; STIC-Biotech/ChemLib

Subject:

RE: RUSH request for 10/047,251

Importance: High

Please rush. Thanks Chris

Chris Chan TC 1600 New Hire Training Coordinator and SPE 1644 (571)-272-0841 Remsen, 3E89

> ----Original Message-----From: Hanley, Susan

Sent: Monday, April 25, 2005 2:11 PM

To: Chan, Christina

Subject: RUSH request for 10/047,251

Christina,

I turned in several searches for 10/047,251 to STIC last week. I really need to get this case out (overdue amended) this biweek. Could you ask for a change to RUSH status for all of the requests that I turned in for this case and forward it to STIC?

Thanks.

Susan Hanley US Patent and Trademark Office Art Unit 1651

Office: Remsen 3D70 Mail Box: Remsen 3E71 Phone: 571-272-2508 => fil hcaplus FILE 'HCAPLUS' ENTERED AT 12:06:15 ON 27 APR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 27 Apr 2005 VOL 142 ISS 18 FILE LAST UPDATED: 26 Apr 2005 (20050426/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que 136

L28 ST

REP G1=(0-1) AK VAR G2=1/2 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE L29 SCR 1840

L31 101049 SEA FILE=REGISTRY SSS FUL L28 AND L29

L35 STR

VAR G1=O/S
VAR G2=O/C
NODE ATTRIBUTES:
CONNECT IS X2 RC AT 12
CONNECT IS X2 RC AT 17
CONNECT IS E1 RC AT 21
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 19
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L36 1 SEA FILE=REGISTRY SUB=L31 SSS FUL L35

REP G1=(0-1) AK VAR G2=1/2 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L29

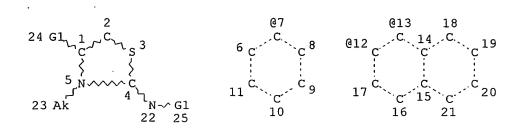
SCR 1840

L31

101049 SEA FILE=REGISTRY SSS FUL L28 AND L29

L37

STR



VAR G1=7/12/13 NODE ATTRIBUTES: CONNECT IS E1 RC AT 23 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 6 12
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L39 4988 SEA FILE=REGISTRY SUB=L31 SSS FUL L37 L43 STR

NODE ATTRIBUTES:
CONNECT IS M1 RC AT 1
CONNECT IS M1 RC AT 4
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L44 4619 SEA FILE=REGISTRY SUB=L39 CSS FUL L43

=> fil caold FILE 'CAOLD' ENTERED AT 12:07:23 ON 27 APR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE

display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d all hitstr 160 1

ANSWER 1 OF 1 CAOLD COPYRIGHT 2005 ACS on STN ANCA60:12019b CAOLD TIthiazolines PA CIBA Ltd. DTPatent PATENT NO. KIND DATE PIBE 627278 DE 1218210 FR 1347371 GB 1027561 1643-94-3 IT 1744-47-4 1800-94-8 1957-57-9 2192-58-7 2677-70-5 90434-86-9 90797-74-3 91066-64-7 91088-92-5 91092-29-4 91566-52-8 93001-25-3 93116-81-5 93190-15-9 91568-29-5 92292-54-1 93284-28-7 93329-91-0 93387-58-7 93439-31-7 93479-33-5 93864-04-1 94095-94-0 94625-57-7 95195-09-8 95750-58-6 95914-19-5 96080-23-8 96750-33-3 97238-53-4 **97554-72-8 98470-56-5** 97554-72-8 98470-56-5 IT 97554-72-8 CAOLD RN CN 4-Thiazoline, 2-[(3,4-dichlorophenyl)imino]-3-methyl-4-phenyl-,

hydrobromide (7CI) (CA INDEX NAME)

• HBr

RN 98470-56-5 CAOLD
CN 4-Thiazoline, 3-isopropyl-4-phenyl-2-(phenylimino)-, hydrobromide (7CI)
(CA INDEX NAME)

HBr

=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 12:08:03 ON 27 APR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 27 Apr 2005 VOL 142 ISS 18 FILE LAST UPDATED: 26 Apr 2005 (20050426/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all hitstr 167 1

L67 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1964:68243 HCAPLUS 60:68243 DN OREF 60:12019b-f ED Entered STN: 22 Apr 2001 Thiazolines TTPA CIBA Ltd. SO 33 pp. DT Patent LΑ Unavailable 38 (Heterocyclic Compounds (More Than One Hetero Atom)) PATENT NO. KIND DATE APPLICATION NO. DATE _____ -----BE 627278 19630718 ΒE DE 1218210 DE FR 1347371 FR GB 1027561 GB

PRAI CH

19620109

```
CLASS PATENT FAMILY CLASSIFICATION CODES
PATENT NO.
     For diagram(s), see printed CA Issue.
GΙ
AΒ
     The title compds. (I) tabulated are prepared by the reaction between a
     monosubstituted thiourea and an \alpha-halocarbonyl compound, and
     eventually alkylation of the formed derivative, or from a N,N'-disubstituted
     thiourea and an \alphahalocarbonyl compound The reaction is effected in
     nonpolar solvents, preferably MePh. I are useful as fungicides,
     bactericides, acaricides, insecticides, and as
     herbicides and weedkillers. To a toluene suspension of
     81.5 g. 3,5-(F3C)2C6H3NHCSNHMe is added, at 90^{\circ} and under stirring,
     25 g. ClCH2COMe. The solution is boiled for 15 min. to give on cooling 65%
     I.HCl [R'= 3,5(F3C)2C6H3, R2 = R3 = Me, R4 = H]; free base m. 87°
     (aqueous EtOH). m.p., m.p.; R1, R2, R3, R4, HCl salt, base; p-ClC6H4, Me, Me,
     H, 193-5°, 67-8°; m-F3CC6H4, Me, Me, H, 189-200°, -; Ph, Me, Me, H, -, 72-4°; 3,4-C12C6H3, Me, Me, H, 193-205°,
     68.5-9.5^{\circ}; CH2:CHCH2, Me, Me, H, -, (b0.04 80^{\circ}); m-F3CC6H4,
     Et, Me, H, 183-93^{\circ}, -; -3,4-Cl2C6H3, Et, Me, H, 170-6^{\circ}, -;
     -3,4-Cl2C6H3, Me, H, H, 191-9°, -; m-F3CC6H4, Me, H, H, -, b0.03
     136-9°); Ph, Me2N, Me, H, 176-91° -; Ph, iso-Pr, Ph, H, (HBr
     salt 196-200°), -; m-MeC6H4, Me, Me, H, -, 48-50°;
     m-ClC6H4, Me, Me, EtO2C, 137-45°, 89-91°; 3,4-Cl2C6H3, Me,
     Me, EtO2C, 137^{\circ}, -; 3,4-Cl2C6H3, Me, H, H, 191-9^{\circ}, -;
     m-ClC6H4, Me, Me, H, 214°, -; o-MeOC6H4, Me, Me, H, 192-5°,
     118-20°; Ph, iso-Pr, Me, H, (perchlorate 148°); -; m-F3CC6H4, H, H, H, 98-107°, -; p-ClC6H4, Me, H, H, 238°, -;
     C12H25, Me, H, H, -, b0.04 148-50°); C12H25, Me, Me, H, -, (b0.03
     130°); p-BrC6H4, Me, Me, H, 211-13°, -; p-BuOC6H4, Me, H, H,
     -, -; p-(p-ClC6H4O)C6H4, Me, Me, H, -, -; 3,4-Cl2C6H3, Me, Ph, H, (HBr
     salt 235-8^{\circ}), -;
     Bactericides, Disinfectants and Antiseptics
IT
         (4-thiazoline derivs. as)
     Fungicides or Fungistats
IT
       Herbicides
       Insecticides
         (4-thiazolines as)
     4-Thiazoline, 3-isopropyl-4-methyl-2-(phenylimino)-, hydrobromide
IT
     6569-17-1, 4-Thiazoline 27394-31-6, 3-Pyrazolidinone,
IT
     4-hydroxy-5-phenyl-
         (derivs.)
     1643-94-3, 4-Thiazoline, 2-[(\alpha,\alpha,\alpha,\alpha',\alpha',\alpha',.al)
     pha.'-hexafluoro-3,5-xylyl)imino]-3,4-dimethyl-
                                                            1744-47-4, 4-Thiazoline,
     3-methyl-2-[(\alpha, \alpha, \alpha-trifluoro-m-tolyl)imino]-
     1800-94-8, 4-Thiazoline, 2-[(\alpha,\alpha,\alpha-trifluoro-m-
     tolyl)imino]-, hydrochloride 1957-57-9, 4-Thiazoline,
     3-\text{ethyl}-4-\text{methyl}-2-[(\alpha,\alpha,\alpha-\text{trifluoro-m-tolyl})\text{imino}]-,
     hydrochloride 2192-58-7, 4-Thiazoline, 2-[(\alpha,\alpha,\alpha,.alph)
     a.',\alpha',\alpha'-hexafluoro-3,5-xylyl)imino]-3,4-dimethyl-,
     hydrochloride 2677-70-5, 4-Thiazoline, 3,4-dimethyl-2-
     [(\alpha, \alpha, \alpha-\text{trifluoro-m-tolyl})] imino]-, hydrochloride
     21257-27-2, Antipyrine, 4-(\alpha-anilinobenzyl)-
                                                         21257-28-3,
     Antipyrine, 4-[\alpha-(p-bromoanilino)benzyl]- 21257-29-4, Antipyrine,
     4-[\alpha-(m-chloroanilino)benzyl]- 90434-86-9, 4-Thiazoline,
     2-(allylimino)-3,4-dimethyl- 90797-74-3, 4-Thiazoline,
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2-[(p-chlorophenyl)imino]-3-methyl- 91066-64-7, 4-Thiazoline, 2-[(p-chlorophenyl)imino]-3,4-dimethyl- 91088-92-5, 4-Thiazoline,

3,4-dimethyl-2-(phenylimino) - 91092-29-4, 4-Thiazoline,

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2-[(3,4-dichlorophenyl)imino]-3,4-dimethyl- 91566-52-8, 4-Thiazoline,
2-[(o-methoxyphenyl)imino]-3,4-dimethyl- 91568-29-5, 4-Thiazoline,
3-ethyl-4-methyl-2-(phenylimino)- 92292-54-1, 4-Thiazoline,
2-[(p-butoxyphenyl)imino]-3-methyl-
                                     93001-25-3, 4-Thiazoline,
3,4-dimethyl-2-(m-tolylimino)- 93116-81-5, 4-Thiazoline,
2-[(3,4-dichlorophenyl)imino]-3-methyl-, hydrochloride
                                                        93190-15-9,
4-Thiazoline, 2-(dodecylimino)-3-methyl- 93284-28-7, 4-Thiazoline,
2-[(p-chlorophenyl)imino]-3,4-dimethyl-, hydrochloride 93329-91-0,
4-Thiazoline, 2-[[p-(p-chlorophenoxy)phenyl]imino]-3,4-dimethyl-
93387-58-7, 4-Thiazoline, 2-[(m-chlorophenyl)imino]-3,4-dimethyl-,
              93439-31-7, 4-Thiazoline, 2-[(p-chlorophenyl)imino]-3-
hydrochloride
methyl-, hydrochloride 93479-33-5, 4-Thiazoline, 2-(dodecylimino)-3,4-
          93864-04-1, 4-Thiazoline-5-carboxylic acid,
dimethyl-
2-[(m-chlorophenyl)imino]-3,4-dimethyl-, ethyl ester
4-Thiazoline, 2-[(p-bromophenyl)imino]-3,4-dimethyl-, hydrochloride
94625-57-7, 4-Thiazoline, 2-[(3,4-dichlorophenyl)imino]-3,4-dimethyl-,
hydrochloride 95195-09-8, 4-Thiazoline, 2-[(3,4-dichlorophenyl)imino]-3-
ethyl-4-methyl-, hydrochloride 95750-58-6, 4-Thiazoline,
2-[(o-methoxyphenyl)imino]-3,4-dimethyl-, hydrochloride. 95914-19-5,
4-Thiazoline-5-carboxylic acid, 2-[(3,4-dichlorophenyl)imino]-3,4-dimethyl-
, ethyl ester, hydrochloride
                             96080-23-8, 4-Thiazoline,
3-(dimethylamino)-4-methyl-2-(phenylimino)-, hydrochloride
                                                            96750-33-3,
4-Thiazoline, 3-isopropyl-4-methyl-2-(phenylimino)-, perchlorate
97238-53-4, 4-Thiazoline-5-carboxylic acid, 2-[(m-chlorophenyl)imino]-3,4-
dimethyl-, ethyl ester, hydrochloride 97554-72-8, 4-Thiazoline,
2-[(3,4-dichlorophenyl)imino]-3-methyl-4-phenyl-, hydrobromide
   (preparation of)
97554-72-8, 4-Thiazoline, 2-[(3,4-dichlorophenyl)imino]-3-methyl-4-
phenyl-, hydrobromide
   (preparation of)
97554-72-8 HCAPLUS
4-Thiazoline, 2-[(3,4-dichlorophenyl)imino]-3-methyl-4-phenyl-,
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IT

RN

CN

• HBr

=> d 168 1,2,4,6,7 bib abs hitstr retable

hydrobromide (7CI) (CA INDEX NAME)

L68 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:492619 HCAPLUS

DN 141:54324

TI Preparation of phenyl carbamates and their use as agrochemical fungicides and insecticides

IN Niki, Toshio; Mizukoshi, Takashi; Suzuki, Hiroyuki; Hayasaka, Fumio

PA Nissan Chemical Industries, Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 78 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

GI

	-						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	JP 2004168706	A2	20040617	JP 2002-336326	20021120		
PRAI	JP 2002-336326		20021120				
os	MARPAT 141:54324						

$$X_{\text{P}}$$
 X_{P}
 X_{P}
 X_{P}
 X_{P}
 X_{P}
 X_{P}

Title compds. I [Ya, Yb = H, halo, C1-6 (halo)alkyl, (un)substituted Ph, (un)substituted heteroaryl; Z = O, S; Z1 = OR1, SR1, NR2R3; B1 = N(OR4), NR5, O, S; X = halo, C1-6 (halo)alkyl, C1-6 alkoxy; R1-R4 = H, C1-6 alkyl; R5 = H, C1-6 (halo)alkyl, C1-6 alkylsulfenyl-C1-6 alkyl, etc.; n = 0-4] or their agriculturally acceptable salts are prepared Thus, 2-[[(dimethylamino)thioxomethyl]amino]-nitrobenzene was treated with 2-bromo-1-(5-trifluoromethyl-1-methylpyrazol-3-yl)-1-propanone, hydrogenated with NaBH4, and condensed with Me chloroformate to give I (Ya = Me, Yb = 5-fluoromethyl-1-methylpyrazol-3-yl, Z = O, Z1COB1 = MeO2CNH, Xn = H), which showed ≥70% antifungal activity against Erysiphe graminis.

IT 481057-15-2P 481062-58-2P 481062-59-3P 481062-62-8P 481062-64-0P 481062-68-4P 481062-70-8P 481062-71-9P 481062-72-0P

Ι

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of Ph carbamates as agrochem. fungicides and insecticides)

RN 481057-15-2 HCAPLUS

CN Carbamic acid, [2-[[4-(2,6-difluorophenyl)-3-methyl-2(3H)-thiazolylidene]amino]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 481062-58-2 HCAPLUS

CN Carbonic acid, methyl 2-[(3-methyl-4-phenyl-2(3H)-

thiazolylidene)amino]phenyl ester (9CI) (CA INDEX NAME)

RN 481062-59-3 HCAPLUS

CN Carbonic acid, 2-[[4-(2-chlorophenyl)-3-methyl-2(3H)-thiazolylidene]amino]phenyl methyl ester (9CI) (CA INDEX NAME)

RN 481062-62-8 HCAPLUS

CN Carbamic acid, [2-[(3-methyl-4-phenyl-2(3H)-thiazolylidene)amino]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 481062-64-0 HCAPLUS

CN Carbamic acid, methyl[2-[(3-methyl-4-phenyl-2(3H)-thiazolylidene)amino]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 481062-68-4 HCAPLUS

CN Carbamic acid, [[2-[(3-methyl-4-phenyl-2(3H)-thiazolylidene)amino]phenyl]m

RN 481062-70-8 HCAPLUS

CN Benzenamine, 2-(1H-imidazol-1-ylmethyl)-N-(3-methyl-4-phenyl-2(3H)-thiazolylidene)- (9CI) (CA INDEX NAME)

RN 481062-71-9 HCAPLUS

CN Benzenamine, N-(3-methyl-4-phenyl-2(3H)-thiazolylidene)-2-(4-morpholinylmethyl)- (9CI) (CA INDEX NAME)

RN 481062-72-0 HCAPLUS

CN Benzenamine, 2-[(hexahydro-1H-azepin-1-yl)methyl]-N-(3-methyl-4-phenyl-2(3H)-thiazolylidene)- (9CI) (CA INDEX NAME)

L68 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:470483 HCAPLUS

DN 139:36541

TI Preparation of heterocyclylimino aromatic compounds as agricultural and horticultural fungicides

IN Niki, Toshio; Mizukoshi, Takashi; Io, Tomoaki; Suzuki, Hiroyuki; Hayasaka, Fumio

PA Nissan Chemical Industries, Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 131 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PRAI	JP 2003171370 JP 2001-193535	A2 A	20030620 20010626	JP 2002-184842	20020625
	JP 2001-299551	Α	20010928		
os	MARPAT 139:36541		•		
GI					

$$\begin{array}{c} V?-V? \\ V? \\ V? \\ V?-V? \end{array}$$

The title compds. (I; Va, Vb, Vc, Vd = C, N, O, or S atom; Ve = C, N, O, or S atom or a single bond; provided that at least one of Va, Vb, Vc, Vd, and Ve is N, O, or S atom; each Va-Vb, Vb-Vc, Vc-Vd, or Vd-Ve is a single or double bond; A2 = naphthyl, heterocyclyl such as substituted pyrazolyl, pyridyl, 3-thienyl, 2-pyrrolyl, 2-imidazolyl, and 1,2,4-triazol-3-yl) are prepared Thus, phenacyl bromide was added to a solution of 2-[1,3-dimethyl-4-[[(methylamino)thioxomethyl]amino]pyrazol-5-yl]acetic acid Me ester in DMF and heated at 80° for 3 h with stirring to give 2-[1,3-dimethyl-4-[(5-methyl-4-phenyl-2,3-dihydro-2-thiazolylidene)amino]pyrazol-5-yl]acetic acid Me ester (II). II at 500 ppm controlled ≥70% Puccinia recondita on wheat seedlings.

IT 544443-58-5P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclylimino aromatic compds. as agricultural

and horticultural fungicides)

RN 544443-58-5 HCAPLUS

CN 1-Naphthaleneacetic acid, 2-[[4-(2,6-difluorophenyl)-3-methyl-2(3H)-thiazolylidene]amino]-, methyl ester (9CI) (CA INDEX NAME)

L68 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:504619 HCAPLUS

DN 137:63241

TI Preparation of 3- or 4-(aminothiazolyl)benzenesulfonamides as parasiticides

IN Fruechtel, Joerg; Koch, Sandra; Newton, Trevor; Miculka, Christian; Mcconnell, Darryl; Hofmann, Joachim

PA Akzo Nobel N.V., Neth.

SO PCT Int. Appl., 25 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

FA	N.CN	1	1																
	PATENT NO.						KIN	D	DATE		APPLICATION NO.						DATE		
								-											
ΡI	V	NO	20020	0514	10		A2 20020704			WO 2001-EP15119						2	00112	219	
	V	O	20020	0514	10		A3		2003	20030731									
			W:	AE,	AG,	AL,	ΑU,	BA,	BB,	BG,	BR,	BZ,	CA,	CN,	co,	CR,	CU,	CZ,	DM,
				DZ,	EC,	EE,	GD,	GE,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	ΚP,	KR,	LC,	LK,
				LR,	LT,	LV,	MA,	MG,	MK,	MN,	MX,	ΜZ,	NO,	ΝZ,	PH,	PL,	RO,	RU,	SG,
				SI,	SK,	SL,	TR,	TT,	UA,	US,	UZ,	VN,	YU,	ZA					
			RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
				KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	CH,	CY,	DE,	DK,	ES,	ΓĮ,	FR,	GB,
				GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,
				GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG							
חח	7 T T	חיד	2000	204	720		70		2000	1222									

PRAI EP 2000-204739 A 20001222

OS MARPAT 137:63241

GΙ

AB R2Z2ZZ1R1 [I; R1 = alk(en)yl, (hetero)aryl, etc.; R2 = Z3NR7R8; R7,R8 = H alkyl, aryl, etc.; Z = (un)substituted thiazole-4,2-diyl; Z1 = bond or (un)substituted imino; Z2 = (un)substituted phenylene; Z3 = bond, CO, SO2] were prepared Thus, 3-(ClO2S)C6H4COCH2Br was cyclocondensed with PhNHCSNH2 and the product amidated by PhCH2NHMe to give title compound II. Data for biol. activity of I were given.

IT 439696-67-0P 439696-69-2P 439696-70-5P 439696-71-6P 439696-72-7P 439696-73-8P 439696-74-9P 439696-75-0P 439696-76-1P 439696-79-4P 439696-80-7P

RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)

(preparation of 3- or 4-(aminothiazolyl)benzenesulfonamides as parasiticides)

RN 439696-67-0 HCAPLUS

CN Benzenesulfonamide, 3-[3-ethyl-2,3-dihydro-2-(phenylimino)-4-thiazolyl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 439696-69-2 HCAPLUS

CN Benzenesulfonamide, 3-[2,3-dihydro-3-methyl-2-(phenylimino)-4-thiazolyl]-N,N-dipropyl-(9CI) (CA INDEX NAME)

RN 439696-70-5 HCAPLUS

CN Benzenesulfonamide, 3-[2,3-dihydro-3-methyl-2-(phenylimino)-4-thiazolyl]-N,N-di-2-propenyl-(9CI) (CA INDEX NAME)

RN 439696-71-6 HCAPLUS

CN Benzenesulfonamide, N-cyclohexyl-3-[2,3-dihydro-3-methyl-2-(phenylimino)-4-thiazolyl]- (9CI) (CA INDEX NAME)

RN 439696-72-7 HCAPLUS

CN Benzenesulfonamide, N-(1,3-benzodioxol-5-ylmethyl)-3-[2,3-dihydro-3-methyl-2-(phenylimino)-4-thiazolyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & O \\ N & NH - CH_2 & O \\ S & NH - CH_2 & O \end{array}$$

RN 439696-73-8 HCAPLUS

CN Benzenesulfonamide, N-[2-[4-(aminosulfonyl)phenyl]ethyl]-3-[2,3-dihydro-3-methyl-2-(phenylimino)-4-thiazolyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & O \\ N & \parallel & S - NH - CH_2 - CH_2 \end{array}$$

RN 439696-74-9 HCAPLUS

CN Benzenesulfonamide, 3-[2,3-dihydro-3-methyl-2-(phenylimino)-4-thiazolyl]-N-(2-thienylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & O & O \\ N & NH - CH_2 \end{array}$$

RN 439696-75-0 HCAPLUS

CN Benzenesulfonamide, 3-[2,3-dihydro-3-methyl-2-(phenylimino)-4-thiazolyl]-N-phenyl- (9CI) (CA INDEX NAME)

RN 439696-76-1 HCAPLUS

CN Benzenesulfonamide, 3-[2,3-dihydro-3-methyl-2-(phenylimino)-4-thiazolyl]-N-(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 439696-79-4 HCAPLUS

CN Isoquinoline, 2-[[3-[2,3-dihydro-3-methyl-2-(phenylimino)-4-thiazolyl]phenyl]sulfonyl]-1,2,3,4-tetrahydro-(9CI) (CA INDEX NAME)

RN 439696-80-7 HCAPLUS

CN Piperazine, 1-[[3-[2,3-dihydro-3-methyl-2-(phenylimino)-4-thiazolyl]phenyl]sulfonyl]-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)

L68 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:116937 HCAPLUS

DN 114:116937

TI Preparation of thiazolines as insecticides and acaricides

IN Nagasaki, Fumihiko; Suzuki, Junji; Ono, Ippei; Yamada, Tomio; Takahashi, Eiko; Hatano, Renpei

PA Nippon Soda Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DT Patent LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	JP 02235877	A2	19900918	JP 1989-55425	19890308
PRAI	JP 1989-55425		19890308		

OS MARPAT 114:116937

GΙ

$$R^{1}N = \begin{pmatrix} S & R^{3} & R^{5} \\ N & Q & R^{6} \\ R^{2} & R^{4} & I \end{pmatrix}$$

AB Insecticides and acaricides contain ≥1 thiazolines I (R1, R2 = lower alkyl, Q; R3, R4 = H, halo-substituted lower alkyl or Ph; R5 = lower alkyl; R6 = H, lower alkyl; X = CHR7; R7 = H, lower alkyl), prepared from R1NHCSNHR2 (II) and YCHR3CR4r1r2 (Y = halo; r1, r2 = lower alkoxy, r1r2 = O) as active ingredients. A solution of 1.9 g II (R1 = Me3C, R2 = 2,6-diisopropyl-4-benzylphenyl) in MeEtCO was refluxed with 1.3 g 1,3-dichloroacetone for 1 h to give 2.1 g I (R1 = Me3C, R2 = 2,6-diisopropyl-4-benzylphenyl, R3 = H, R4 = CH2Cl) (III). III 20, higher alc. sulfate esters 5, diatomaceous earth 70, and white carbon 5 parts were mixed to give a wettable powder, which was applied at 125 ppm to sweet potato leaves to result in 100% insecticidal effect against Spodoptera litura.

IT 132570-40-2 132570-41-3 132570-42-4

132570-43-5 132570-44-6

RL: BIOL (Biological study)

(agrochem. insecticides and acaricides containing, preparation of)

RN 132570-40-2 HCAPLUS

CN Benzenamine, N-[4-(4-chlorophenyl)-3-methyl-2(3H)-thiazolylidene]-2,6-bis(1-methylethyl)-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 132570-41-3 HCAPLUS

CN Benzenamine, N-[4-(4-chlorophenyl)-3-ethyl-2(3H)-thiazolylidene]-2,6-bis(1-methylethyl)-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$i-Pr$$
 N
 $i-Pr$
 CH_2-Ph

RN 132570-42-4 HCAPLUS

CN Benzenamine, N-[4-(2,4-dichlorophenyl)-3-methyl-2(3H)-thiazolylidene]-2,6-bis(1-methylethyl)-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
Me & i-Pr \\
\hline
N & N
\end{array}$$

$$\begin{array}{c|c}
CH_2-Ph \\
\end{array}$$

RN 132570-43-5 HCAPLUS

CN Benzenamine, N-[4-(2,4-dichlorophenyl)-3-ethyl-2(3H)-thiazolylidene]-2,6-bis(1-methylethyl)-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{i-Pr} \\ & \text{N} \\ & \text{N} \\ & \text{C1} \\ & \text{i-Pr} \\ & \text{CH}_2\text{-Ph} \\ \end{array}$$

RN 132570-44-6 HCAPLUS

CN Benzenamine, N-[4-(2,4-dichlorophenyl)-3-(1-methylethyl)-2(3H)-thiazolylidene]-2,6-bis(1-methylethyl)-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$i-Pr$$
 $i-Pr$
 N
 N
 $C1$
 $i-Pr$
 CH_2-Ph

L68 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1989:192810 HCAPLUS

DN 110:192810

TI Preparation of thiazoline derivatives as acaricides and insecticides

PA Nippon Soda Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	JP 63250371	A2	19881018	JP 1987-82455	19870403
	JP 07116168	B4	19951213		
PRA	I JP 1987-82455		19870403		
os	MARPAT 110:192810				
GΙ					

$$R^3$$
 R^4
 S
 NR^2
 R^5
 XR^7
 R^6
 XR^7

Title compds. I [R1, R2 = (Ph-substituted) alkyl, cycloalkyl, Q wherein R5 = alkyl, alkylamino, R6 = H, alkyl, alkylamino, R7 = (halo- or haloalkyl-substituted) Ph or pyridyl; X = O, S; at least one of R1 and R2 = Q; R3, R4 = H, halo, (halo-substituted) alkyl or Ph] are prepared by cyclocondensation of R1NHC(:S)NHR2 with R3CHX1CR4R8R9 (X1 = halo; R8, R9 = alkoxy or R1R2 = O). A solution of C1CH2COMe and 2,6,4-Me2(PhO)C6H2NHC(:S)NHCMe3 in EtCOMe was refluxed to give I [R1 = Me3C; R2 = 2,6,4-Me2(PhO)C6H2; R3 = H; R4 = Me], which at 125 ppm showed 100% control of imagoes of Tetranycus urticae, vs. 0% for a known I [R1 = p-(p-C1C6H4O)C6H4; R2 = R4 = Me; R3 = H]. An emulsion was formulated containing I 10, alkyl phenyl polyoxyethylene 5, DMF 50, and xylene 35 parts.

IT 120258-91-5P 120258-92-6P 120258-93-7P 120258-94-8P 120258-95-9P 120258-98-2P 120258-99-3P 120259-00-9P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as insecticide and acaricide)

RN 120258-91-5 HCAPLUS

CN Benzenamine, 2,6-bis(1-methylethyl)-N-(3-methyl-4-phenyl-2(3H)-thiazolylidene)-4-phenoxy-(9CI) (CA INDEX NAME)

RN 120258-92-6 HCAPLUS

CN Benzenamine, N-(3-ethyl-4-phenyl-2(3H)-thiazolylidene)-2,6-bis(1-methylethyl)-4-phenoxy- (9CI) (CA INDEX NAME)

RN 120258-93-7 HCAPLUS

CN Benzenamine, 2,6-bis(1-methylethyl)-4-phenoxy-N-(4-phenyl-3-propyl-2(3H)-thiazolylidene)- (9CI) (CA INDEX NAME)

RN 120258-94-8 HCAPLUS

CN Benzenamine, 2,6-bis(1-methylethyl)-N-[3-(1-methylethyl)-4-phenyl-2(3H)-thiazolylidene]-4-phenoxy- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
i-Pr & i-Pr \\
\hline
Ph & N & \\
S & \\
i-Pr & OPh
\end{array}$$

RN 120258-95-9 HCAPLUS

CN Benzenamine, 2,6-bis(1-methylethyl)-N-[3-(1-methylpropyl)-4-phenyl-2(3H)-thiazolylidene]-4-phenoxy- (9CI) (CA INDEX NAME)

RN 120258-98-2 HCAPLUS

CN Benzenamine, N-[4-(4-chlorophenyl)-3-(1-methylethyl)-2(3H)-thiazolylidene]-2,6-bis(1-methylethyl)-4-phenoxy-(9CI) (CA INDEX NAME)

- RN 120258-99-3 HCAPLUS
- CN Benzenamine, N-[4-(2,3-dichlorophenyl)-3-methyl-2(3H)-thiazolylidene]-2,6-bis(1-methylethyl)-4-phenoxy- (9CI) (CA INDEX NAME)

- RN 120259-00-9 HCAPEUS
- CN Benzenamine, N-[4-(2,3-dichlorophenyl)-3-(1-methylethyl)-2(3H)-thiazolylidene]-2,6-bis(1-methylethyl)-4-phenoxy-(9CI) (CA INDEX NAME)

- => d 168 3,5 bib abs hitrn fhitstr retable
- L68 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
- AN 2003:5930 HCAPLUS
- DN 138:73261
- TI Preparation of heterocyclyliminophenyl compounds as agricultural and horticultural fungicides and insecticides
- IN Niki, Toshio; Mizukoshi, Takashi; Takahashi, Hiroaki; Satow, Jun; Ogura, Tomoyuki; Yamagishi, Kazuhiro; Suzuki, Hiroyuki; Hayasaka, Fumio
- PA Nissan Chemical Industries, Ltd., Japan
- SO PCT Int. Appl., 508 pp. CODEN: PIXXD2
- DT Patent
- LA Japanese

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PΤ
    WO 2003000659
                               20030103
                                           WO 2002-JP6424
                                                                  20020626
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT,
            LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT,
            RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG,
            US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
            CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                               20040108
    JP 2004002250
                         A2
                                          JP 2002-184667
                                                                  20020625
PRAI JP 2001-192285
                         Α
                               20010626
    JP 2001-193428
                         Α
                               20010626
    JP 2001-385120
                         Α
                               20011218
    JP 2001-386846
                               20011220
                         Α
                               20020328
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JP 2002-90213 OS MARPAT 138:73261

GI

$$A=N$$
 G
 $(X)_n$

AB The title compds. I [A is an optionally substituted heterocycle; X is hydrogen or the like; and G is CH2COOMe, N(Me)COOMe, or the like; n = 0 -4] are prepared Compds. of this invention at 500 ppm gave ≥ 70% control of Pyricularia oryzae.

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TΤ
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     347874-06-0P 347874-07-1P 347874-08-2P
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Ι

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481062-72-0P 481062-74-2P
RL: AGR (Agricultural use); BSU (Biological study,
unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP
(Preparation); USES (Uses)
   (preparation of heterocyclyliminophenyl compds. as agricultural
   and horticultural fungicides and insecticides)
481065-52-5P 481065-53-6P 481065-54-7P
481065-55-8P 481065-57-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation of heterocyclyliminophenyl compds. as agricultural
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IT

and horticultural fungicides and insecticides)

IT 347871-82-3P

RL: AGR (Agricultural use); BSU (Biological study,

unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP
(Preparation); USES (Uses)

(preparation of heterocyclyliminophenyl compds. as agricultural and horticultural fungicides and insecticides)

RN 347871-82-3 HCAPLUS

CN Benzeneacetic acid, 2-[(3-methyl-4-phenyl-2(3H)-thiazolylidene)amino]-,
 methyl ester (9CI) (CA INDEX NAME)

RETABLE

Referenced Author	Year VOL	PG	Referenced Work	Referenced
(RAU)	(RPY) (RVL)	(RPG)	(RWK)	File
	+====+====	+=====	=+===========	=+=========
Boots Co Plc	1990		JP 02229148 A	HCAPLUS
Boots Co Plc	1990	1	GB 2226562 A1	HCAPLUS
Boots Co Plc	1990		EP 385038 A1	HCAPLUS
Boots Co Plc	1990		US 5223498 A	HCAPLUS
Boots Co Plc	1990		US 5373008 A	HCAPLUS
Dai Nippon Printing Co	1991		JP 03-16792 A	HCAPLUS
Dai Nippon Printing Co	1991		US 5021394 A	HCAPLUS
Fuji Photo Film Co Ltd	1993		JP 03-244593 A	HCAPLUS
Fuji Photo Film Co Ltd	1993		JP 05-177959 A2	HCAPLUS
Fuji Photo Film Co Ltd	1993		JP 05-202305 A	HCAPLUS
Fuji Photo Film Co Ltd	1993	1	JP 05-70704 A	HCAPLUS
Fuji Photo Film Co Ltd	1993		US 5238903 A	HCAPLUS
Kalcheva, V	1993	1319	Liebigs Ann Chem	HCAPLUS
Nissan Chemical Industr	2001		WO 0147888 A1	HCAPLUS
Sumitomo Chemical Co Lt	1988	1	JP 01-165565 A	HCAPLUS
Sumitomo Chemical Co Lt	1988	1	EP 287377 A2	HCAPLUS
Sumitomo Chemical Co Lt	1988	1	US 5028708 A	HCAPLUS
Sumitomo Chemical Co Lt	1988		US 5061796 A	HCAPLUS
Sumitomo Chemical Co Lt	1988	1	US 5136054 A	HCAPLUS
Sumitomo Chemical Co Lt	1988	1	US 5220027 A	HCAPLUS

L68 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:489370 HCAPLUS

DN 135:76866

TI Preparation of heterocyclic imino compounds as fungicides and insecticides for agricultural and horticultural use

IN Niki, Toshio; Mizukoshi, Takashi; Takahashi, Hiroaki; Satow, Jun; Ogura, Tomoyuki; Yamagishi, Kazuhiro; Suzuki, Hiroyuki; Hayasaka, Fumio

PA Nissan Chemical Industries, Ltd., Japan

SO PCT Int. Appl., 350 pp. CODEN: PIXXD2

DT Patent

PAN.	~IN I	T																		
	PAT	CENT 1	NO.			KIN	D ·	DATE			APPL	ICAT	ION :	NO.		DATE				
DT		2001	0470				-	2001	0705	WO 2000-JP9411							00001000			
PΙ	WO																			
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									KZ,					•	•	•	·	•		
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									GR,											
									GN,							-	,	,		
	ΑU	2001	-	-	-	-	•				-	•	•	•	•		0001	228		
										EP 2000-985987										
									FR,											
				•		-			MK,				,	,	,	,	,	,		
	US	2003							1113				1689	68		2	0020	625		
PRAT		1999							1228							_	0020			
	.TP	2000	-239	624		Δ														
		2000																		
		2000																		
						VV		2000	1220											
os	MAI	RPAT :	135:	1686	ь															
GI																				

$$A=N$$
 G
 I
 Me
 Me
 Me
 $(X)_{n}$
 I
 $H_{2}C-CO-OMe$

AB The title compds. I [G is a group of general formula BCOZ or the like; A is a 3- to 13-membered, mono-, di- or tricyclic ring which is composed of 3 to 13 atoms arbitrarily selected from among carbon, oxygen, sulfur and nitrogen, contains at least one heteroatom selected from among oxygen, sulfur and nitrogen, and may optionally have substituent(s), with the proviso that when A is a quinolone ring, the nitrogen atom of the ring is present at the α-position to the imino linkage; Z is OR1 or the like; B is CH2 or the like; n = 0 - 4; X is halogeno or the like; and R1 is hydrogen, C1-6 alkyl, C1-6haloalkyl, or the like) are prepared The title compound II at 500 ppm gave ≥ 70% control of Pyricularia oryzae, Erysiphe graminis, Puccinia recondita, Leptosphaera nodorum, and Pseudoperonospora cubensis. II at 500 ppm gave ≥ 70% control of

II

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leafhoppers.
IT
     347871-82-3P 347871-85-6P 347871-89-0P
     347871-92-5P 347871-95-8P 347871-97-0P
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     347876-18-0P 347876-19-1P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
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BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of heterocyclic imino compds. as fungicides and insecticides for agricultural and horticultural use)

IT 347871-82-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic imino compds. as fungicides and insecticides for agricultural and horticultural use)

RN 347871-82-3 HCAPLUS

CN Benzeneacetic acid, 2-[(3-methyl-4-phenyl-2(3H)-thiazolylidene)amino]-, methyl ester (9CI) (CA INDEX NAME)

RETABLE

Referenced Author (RAU)	(RPY)	VOL (RVL)	(RPG)	Referenced Work (RWK)	Referenced File
Geigy J R A-G	-+ 	 	 	FR 1601535 A	HCAPLUS
Geigy J R A-G	1	1		DE 1816700 C3	HCAPLUS
Geigy J R A-G	11971	1	l	GB 1258920 A	HCAPLUS
Maeda, R	11983	31	3424	Chem Pharm Bull	HCAPLUS
Nissan Chemical Industr	11994		1	JP 06157478 A	HCAPLUS
Toa Wool Spinning & Wea	a 1995		1	JP [.] 753527 A	
Werbel, L	1969	12	521	J Med Chem	HCAPLUS

=> d 169 bib abs hitstr retable 1-7

L69 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2005:141200 HCAPLUS

DN 142:254568

TI Methods and compositions for increasing the efficacy of biologically-active ingredients such as antitumor agents

IN Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan
M.; Thomas, Collin E.

PA Board of Regents, the University of Texas System, USA

SO PCT Int. Appl., 243 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT	KIND DATE				APPL	ICAT		DATE								
	WO 2005014777					_											
ΡI					A2	A2 2005				WO 2003-US32667						20031016	
	W:	ΑĒ,	ΑG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	GE,
		GH.	GM.	HR.	HU.	ID.	IL.	IN.	IS.	JP.	KE.	KG.	KP.	KR.	KZ.	LC.	LK.

LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI US 2002-418803P

P 20021016

AB The invention provides methods and compns. for modulating the sensitivity of cells to cytotoxic compds. and other active agents. In accordance with the invention, compns. are provided comprising combinations of ectophosphatase inhibitors and active agents. Active agents include antibiotics, fungicides, herbicides, insecticides, chemotherapeutic agents, and plant growth regulators. By increasing the efficacy of active agents, the invention allows use of compns. with lowered concns. of active ingredients.

IT 291536-79-3 291536-90-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)

(methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

RN 291536-79-3 HCAPLUS

CN Benzenamine, N-(3-hexyl-4-phenyl-2(3H)-thiazolylidene)-, monohydrobromide (9CI) (CA INDEX NAME)

HBr

RN 291536-90-8 HCAPLUS

CN 4-Thiazolidinone, 3-[[(4-methoxyphenyl)amino]methyl]-2-methylene-5-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

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L69 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
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AN 2003:23438 HCAPLUS

DN 138:68713

TI Modulating resistance of tumor and pathogen cells to foreign compounds by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases

IN Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan

PA University of Texas, USA

SO U.S. Pat. Appl. Publ., 41 pp., Cont.-in-part of U.S. Ser. No. 261,825. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 3

FAN.	PATENT	NO.	KI	KIND DATE				APPLICATION NO.						DATE		
PI	US 2003	3008369	 A	A1 20030109			1	US 2002-134019								
	US 2002006901			A1 20020117			1	US 1999-244792						19990205		
	WO 2003	3091403	A	A2 20031106			1	WO 2003-US12780					20030425			
	WO 2003	3091403	Α	A3 20041104												
	W:	AE, AG,	AL, AM	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
		CO, CR,	CU, CZ	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM, HR,	HU, ID	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	
		LS, LT,	LU, LV	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,	
		PH, PL,	PT, RO	, RU,	SC,	SD,	SE,	SG,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	
		TZ, UA,	UG, US	, UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW						
	RW:	GH, GM,	KE, LS	, MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪG,	ZM,	ZW,	AM,	AZ,	BY,	
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		FI, FR,	GB, GR	, HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,	
		BF, BJ,	CF, CG	, CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
PRAI	US 1999	9-244792	A	2	1999	0205	•	~.	•	•	•	•	•	•		
	US 1999	9-261825	A	2	1999	0303										

US 2002-134019 A1 20020425

The present invention relates to methods for modulating the growth of tumor and pathogen cells and the resistance of cells to foreign compds., i.e. drugs, antibiotics, etc. by altering the ATP gradient across biol. membranes. The altering of the ATP gradient across biol. membranes is achieved through the manipulation of ecto-phosphatase (e.g., human apyrase) activity and ABC transporter mol. (e.g., Arabidopsis AtPGP-1) activity which may also be useful to confer herbicide resistance to plants, confer antibiotic resistance to bacteria, confer drug resistance to yeast cells, or to reduce resistance in cells to facilitate chemotherapeutic treatments, and to reduce resistance in bacteria and yeast. The present invention is also directed to the methods for identifying ecto-phosphatase inhibitors and uses thereof.

Nineteen ecto-phosphatase inhibitory mols. are provided which are useful in reversing multi-drug resistance in Arabidopsis and yeast.

IT 291536-79-3 291536-90-8

RL: AGR (Agricultural use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

RN 291536-79-3 HCAPLUS

CN Benzenamine, N-(3-hexyl-4-phenyl-2(3H)-thiazolylidene)-, monohydrobromide (9CI) (CA INDEX NAME)

HBr

RN 291536-90-8 HCAPLUS

CN 4-Thiazolidinone, 3-[[(4-methoxyphenyl)amino]methyl]-2-methylene-5-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

IT 9013-05-2, Phosphatase

RL: BSU (Biological study, unclassified); BIOL (Biological study) (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

RN 9013-05-2 HCAPLUS

CN Phosphatase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L69 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:833490 HCAPLUS

DN 137:306061

TI Pesticidal and herbicidal activity through modulation of animal and plant cell membrane transport

IN Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan
M

PA Board of Regents, The University of Texas System, USA

SO U.S. Pat. Appl. Publ., 41 pp., Cont.-in-part of U.S. Ser. No. 244,791. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 2002160915	A1	20021031	US 2001-793336	20010226	
	US 6448472	В1	20020910	US 1999-244791	19990205	
PRAI	US 1999-244791	A2	19990205			
	US 2000-185299P	P	20000228		•	

AB The present invention relates to the modulation of pesticidal and herbicidal activity by treatment of a membrane transport system in a cell. This entails modifying the extra-cellular phosphatases found in the membranes of these cells. By modifying

the ATP gradient across the biol. membrane of a target plant, bacteria, insect or mammalian cell via inhibiting one or more extra-cellular phosphatases, it is possible to alter the sensitivity to a pesticide or herbicide. The method also comprises inhibiting an ABC transporter in the target cell. The method can also be used for identifying chems. with pesticidal activity.

IT 291536-79-3 291536-90-8

RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(ectophosphatase inhibitor which enhances pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes)

RN 291536-79-3 HCAPLUS

CN Benzenamine, N-(3-hexyl-4-phenyl-2(3H)-thiazolylidene)-, monohydrobromide (9CI) (CA INDEX NAME)

HBr

RN 291536-90-8 HCAPLUS

CN 4-Thiazolidinone, 3-[[(4-methoxyphenyl)amino]methyl]-2-methylene-5-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

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IT
     9032-64-8, Nucleotide pyrophosphatase 37289-25-1
     , ATP pyrophosphatase
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (extracellular; ectophosphatase inhibitors which enhance
        pesticidal and herbicidal activity by altering the
        ATP gradient across biol. membranes)
RN
     9032-64-8 HCAPLUS
     Pyrophosphatase, nucleotide (9CI) (CA INDEX NAME)
CN
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     37289-25-1 HCAPLUS
RN
     Pyrophosphatase, adenosine triphosphate (9CI) (CA INDEX NAME)
CN
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
L69
     2002:185280 HCAPLUS
ΑN
DN
     136:244034
ΤI
     Method for increasing the effectiveness of antiinfective agents by
     inhibiting ecto-phosphatase and/or ABC transporter activities
     Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan
IN
     Board of Regents, the University of Texas System, USA
PΑ
SO
     PCT Int. Appl., 65 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                  DATE
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                                                                        DATE
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     WO 2002020726
                          A2
                                  20020314
                                               WO 2001-US28242
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              LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
              PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
             US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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                                  20020322
                                             AU 2001-90710
                                                                        20010907
     AU 2001090710
                           Α5
                                              US 2001-949268
     US 2002077365
                           A1
                                  20020620
                                                                        20010907
PRAI US 2000-231088P
                           Ρ
                                  20000908
     WO 2001-US28242
                           W
                                  20010907
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GΙ

Ι

- AB The present invention relates to methods for decreasing the resistance of microbial strains to antiinfectives such an antibiotics and antifungals by altering the ATP gradient across biol. membranes. The altering of the ATP gradient across biol. membranes is achieved through the inhibition of ecto-phosphatase activity and/or ABC transporter mol. activity which may be useful to reduce resistance in bacteria and yeast to aid in the treatment of certain infections and disease and to lower the concentration
- of
 antiinfectives necessary to inhibit the growth of microbial strains.
 Apyrase inhibitor I increased the growth inhibitory effect of the fungicide chlorothalonil by over 50%. Surflan was an equally effective weed killer against Arabidopsis thaliana at a five-fold less concentration in the presence of II.
- IT 291536-79-3 291536-90-8
 RL: BSU (Biological study, unclassified); CST (Combinatorial study, unclassified); BIOL (Biological study); CMBI (Combinatorial study) (as apyrase inhibitor; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities)
- RN 291536-79-3 HCAPLUS
 CN Benzenamine, N-(3-hexyl-4-phenyl-2(3H)-thiazolylidene)-, monohydrobromide
 (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{(CH2)} 5^{-} \text{Me} \\ \\ \text{Ph-N} \end{array}$$

HBr

RN 291536-90-8 HCAPLUS

CN 4-Thiazolidinone, 3-[[(4-methoxyphenyl)amino]methyl]-2-methylene-5-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

IT 9000-83-3, ATPase

RL: BSU (Biological study, unclassified); BIOL (Biological study) (inhibition of, of ectophosphatase; method for increasing effectiveness of antiinfective agents by inhibiting ectophosphatase and/or ABC transporter activities)

RN 9000-83-3 HCAPLUS

CN Phosphatase, adenosine tri- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L69 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:676991 HCAPLUS

DN 135:222868

TI Pesticide adjuvant activity through modulation of animal and plant cell membrane transport

IN Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.

PA Board of Regents of the University of Texas System, USA

SO PCT Int. Appl., 76 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

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HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
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             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU,
             ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     US 2002103082
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                                                                    20010306
     CA 2373424
                          AA
                                20010913
                                            CA 2001-2373424
                                                                    20010307
PRAI US 2000-187819P
                          Р
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     US 2001-800327
                          Α
                                20010306
     WO 2001-US7423
                          W
                                20010307
```

AB The invention relates to the modulation of pesticidal and herbicidal activity by treatment of a membrane transport system in a cell. This entails modifying the extracellular phosphatases found in the membranes of these cells. By modifying the ATP gradient across the biol. membrane of a target plant, bacteria, insect or mammalian cell via inhibiting one or more extracellular phosphatases, it is possible to alter the sensitivity to a pesticide or herbicide. In preferred embodiments, the chemical moieties of the invention act as adjuvants to enhance pesticidal activity.

IT 9013-05-2, Phosphatase

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(ecto-; pesticide adjuvants acting by inhibition of extracellular phosphatases in membranes)

RN 9013-05-2 HCAPLUS

CN Phosphatase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 291536-79-3 291536-90-8

RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses) (pesticide adjuvant acting by inhibition of extracellular phosphatases in membranes)

RN 291536-79-3 HCAPLUS

CN Benzenamine, N-(3-hexyl-4-phenyl-2(3H)-thiazolylidene)-, monohydrobromide (9CI) (CA INDEX NAME)

HBr

RN 291536-90-8 HCAPLUS

CN 4-Thiazolidinone, 3-[[(4-methoxyphenyl)amino]methyl]-2-methylene-5-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

RETABLE

Referenced Author (RAU)	(RPY) (RVL) (RPG	Referenced Work 	Referenced File -+
Boyum	1997 230 22	Biochem Biophys Res	•
Decottignies	1998 273 1261	2 J Biol Chem	HCAPLUS
Grant	1994 54 357	Cancer Research	HCAPLUS
Thomas	2000 12 519	The Plant Cell	HCAPLUS
University Of Texas	2000	WO 0052144 A1	HCAPLUS

L69 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:661570 HCAPLUS

DN 135:206922

TI Pesticidal and herbicidal activity through modulation of animal and plant cell membrane transport

IN Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan
M.

PA Board of Regents, the University of Texas System, USA

SO PCT Int. Appl., 74 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 3

LAM.	CMI	3																
	PA'	TENT 1	NO.	•		KIND DATE		APPLICATION NO.					DATE					
							-											
ΡI	WO 2001064859				A1 20010907			WO 2001-US6503					20010227					
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
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			HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,
			LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	ΜX,	MZ,	NO,	ΝZ,	PL,	PT,	RO,	RU,
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DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-185299P P 20000228

AB The invention relates to the modulation of pesticidal and herbicidal activity by treatment of a membrane transport system in a cell. This entails modifying the extra-cellular phosphatases found in the membranes of these cells. By modifying the ATP gradient across the biol. membrane of a target plant, bacteria, insect or mammalian cell via inhibiting one or more extracellular phosphatases, it is possible to alter the sensitivity to a pesticide or herbicide. The method also comprises inhibiting an ABC transporter in the target cell. The method can also be used for identifying chems. with pesticidal activity.

IT 291536-79-3 291536-90-8

RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(ectophosphatase inhibitor which enhances pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes)

RN 291536-79-3 HCAPLUS

CN Benzenamine, N-(3-hexyl-4-phenyl-2(3H)-thiazolylidene)-, monohydrobromide (9CI) (CA INDEX NAME)

HBr

RN 291536-90-8 HCAPLUS

CN 4-Thiazolidinone, 3-[[(4-methoxyphenyl)amino]methyl]-2-methylene-5-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

IT 9032-64-8, Nucleotide pyrophosphatase 37289-25-1

, ATP pyrophosphatase

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(extracellular; ectophosphatase inhibitors which enhance pesticidal and herbicidal activity by altering the

ATP gradient across biol. membranes)

RN 9032-64-8 HCAPLUS

CN Pyrophosphatase, nucleotide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 37289-25-1 HCAPLUS

CN Pyrophosphatase, adenosine triphosphate (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RETABLE

Referenced Author (RAU)	Year VOL (RPY) (RVL)	(RPG)	Referenced Work (RWK) +====================================	Referenced File
Lu, Y Thomas, C	1998 10	267	The Plant Cell The Plant Cell	HCAPLUS HCAPLUS

L69 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:628251 HCAPLUS

DN 133:219782

TI Genetic and epigenetic manipulation of ABC transporters and ectophosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors

IN Thomas, Collin E.; Windsor, J. Brian; Roux, Stan
J.; Lloyd, Alan M.; Hurley, Laurence

PA University of Texas, USA

SO PCT Int. Appl., 85 pp.

CODEN: PIXXD2

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DT
     Patent
LA English
FAN.CNT 3
     PATENT NO.
                        KIND
                                DATE
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PΙ
    WO 2000052144
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                                           WO 2000-US5315
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                             20020313 EP 2000-913685
     EP 1185623
                         A1
                                                                  20000228
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     US 2002173031
                                20021121
                                           US 2002-47251
                                                                  20020114
                         A1
PRAI US 1999-261825
                                19990303
                         Α
    WO 2000-US5315
                         W
                                20000228
AΒ
     The present invention relates to methods for modulating the resistance of
     cells to foreign compds., i.e. drugs, antibiotics, etc. by altering the
    ATP gradient across biol. membranes. Altering the ATP gradient across
    biol. membranes is achieved through the manipulation of ecto-
    phosphatase activity and ABC transporter mol. activity. The above
    method may be useful to confer herbicide resistance to
    plants, antibiotic resistance to bacteria, and drug resistance to
    yeast cells, or to reduce resistance in cells, bacteria, and yeast in order
     to facilitate chemotherapeutic treatments. The present invention is also
    directed to the methods for identifying ecto-phosphatase
     inhibitors and uses thereof. Thus, Arabidopsis thaliana has been shown to
    possess an ecto-apyrase and this ecto-apyrase and PGP-1 (an MDR-like
    protein) to have a role in MDR. Addnl., the extracellular ATP pool was
    shown to be critical for MDR in yeast. Screening of a combinatorial library
    of small mols. has resulted in identification of apyrase inhibitors.
IT
     9013-05-2, Phosphatase 291536-79-3
     291536-90-8
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); BIOL (Biological study)
        (genetic and epigenetic manipulation of ABC transporters and ecto-
       phosphatases for modulating drug resistance and methods for
       detection of ecto-phosphatase inhibitors)
RN
     9013-05-2 HCAPLUS
CN
     Phosphatase (9CI) (CA INDEX NAME)
   STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN
     291536-79-3 HCAPLUS
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CN Benzenamine, N-(3-hexyl-4-phenyl-2(3H)-thiazolylidene)-, monohydrobromide (9CI) (CA INDEX NAME)

• HBr

RN 291536-90-8 HCAPLUS

CN 4-Thiazolidinone, 3-[[(4-methoxyphenyl)amino]methyl]-2-methylene-5-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

RETABLE

Referenced Author (RAU)	Year VOL PO (RPY) (RVL) (R	PG) (RWK)	Referenced File
Decottignies Dudler Grant Kiba Lu Sidler Thomas	· ·	7 Cancer Research 9 Plant Cell Physiol 7 The Plant Cell 32 The Plant Cell	HCAPLUS HCAPLUS HCAPLUS HCAPLUS HCAPLUS HCAPLUS
Wang	1996 271 989	•	HCAPLUS

=> d 170 bib abs hitrn fhitstr retable 1-16

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ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
L70
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AN
     137:93746
DN
     2-Arylimino-2,3-dihydrothiazoles, processes for their preparation, and
ΤI
     their use as somatostatin receptor ligands
IN
     Moinet, Christophe; Sackur, Carole; Thurieau, Christophe
PA
     Societe De Conseils De Recherches Et D'applications Scientifiques
     (S.C.R.A.S.), Fr.
     PCT Int. Appl., 465 pp.
SO
     CODEN: PIXXD2
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LA
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     PATENT NO.
                            KIND
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                                                 APPLICATION NO.
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              PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
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          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
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                                    20031022
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     EP 1353912
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              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
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     MARPAT 137:93746
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

GΙ

The invention concerns novel 2-arylimino-2,3-dihydrothiazole derivs. I and their racemates, enantiomers, combinations, and salts [wherein Rl = (un)substituted, particularly amino-substituted alk(en/yn)yl, (hetero)aryl, aralkyl, cycloalkyl, etc.; R2 = (un)substituted carbocyclic or heterocyclic aryl; R3 = alkyl, adamantyl, (un)substituted (hetero)aryl or (hetero)aralkyl, (un)substituted carbamoyl; R4 = H, alkyl, (un)substituted (hetero)aralkyl, etc.]. Also disclosed are methods of their preparation and their use as medicines, in particular for treating a wide variety of pathol. conditions or diseases involving somatostatin receptors. In particular, these pathol. conditions include acromegaly, pituitary adenoma, endocrine gastroenteropancreatic tumors (including carcinoid syndrome), and gastrointestinal bleeding. Examples include a few detailed syntheses, a listing of over 2800 characterized invention

compds., and various precursor prepns. For instance, 4-H2NC6H4CH2CH2NH2 was bound to Wang resin p-nitrophenylcarbonate (at the aliphatic amino group), and the resin-bound amine reacted sequentially with PhCH2CH2NCS, bromopyruvic acid, and 4-ClC6H4CH2NH2 to give, after acidic cleavage, (Z)-isomeric title compound II. Twenty selected compds. I, including III.2HCl, inhibited binding of [125I-Tyr11]SRIF-14 to human somatostatin receptors in vitro with Ki < 200 nM.

TT 322740-74-9P 322740-76-1P 322740-77-2P 322740-78-3P 322740-79-4P 322740-80-7P 322741-53-7P 322741-54-8P 322741-55-9P 322741-56-0P 322741-62-8P 322741-63-9P 322741-64-0P 322741-65-1P 322741-66-2P 322742-27-8P

322742-25-6P 322742-26-7P 322742-27-8P 322742-28-9P 322742-29-0P 322742-30-3P 322742-31-4P 322743-27-1P 322743-28-2P 322743-29-3P 322743-30-6P 322743-31-7P

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of (arylimino)dihydrothiazoles as somatostatin receptor ligands)

IT 322740-74-9P

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of (arylimino)dihydrothiazoles as somatostatin receptor ligands)

RN 322740-74-9 HCAPLUS

CN Benzeneethanamine, 4-[[3-(2-methylpropyl)-4-phenyl-2(3H)-thiazolylidene]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{i-Bu} & \text{CH}_2\text{-}\text{CH}_2\text{-}\text{NH}_2 \\ \\ \text{Ph} & \text{N} & \text{S} & \text{N} \end{array}$$

RETABLE

(RAU)	Year VOL (RPY) (RVL)	(RPG)	Referenced Work (RWK) +===========	Referenced File
Ciba S A Hoechst Ag Omar, A Thurieau, C Wermuth, C	1964 1981	 1166 	FR 1347371 A EP 0023964 A JOURNAL OF PHARMACEU WO 0107424 A	 HCAPLUS

L70 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:165042 HCAPLUS

DN 136:216746

TI Preparation and use of, e.g., 2-arylimino-1,3-thiazolidines as progesterone receptor binding ligands

IN Dixon, Brian R.; Bagi, Cedo M.; Brennan, Catherine R.; Brittelli, David
R.; Bullock, William H.; Chen, Jinshan; Collibee, William L.; Dally,
Robert; Johnson, Jeffrey S.; Kluender, Harold C. E.; Lathrop, William F.;

Liu, Peiying; Mase, Carol Ann; Redman, Aniko M.; Scott, William J.; Urbahns, Klaus; Wolanin, Donald J.

PA Bayer Corp., USA

so U.S., 148 pp.

CODEN: USXXAM

DT Patent

LA English

FAN. CNT 1

rau.	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6353006	B1	20020305	US 1999-453613	19991203
	US 2003207865	A1	20031106	US 2001-4306	20011023
PRAI	US 1999-287573P	P	19990114		
	US 1999-453613	A3	19991203		
os	MARPAT 136:216746				
GI					•

Ι

$$(T)_{t}R \\ N \\ (Q)_{q}R^{2} \\ (Q)_{q}R^{3} \\ (Q)_{q}R^{4} \\ (C_{n}H_{2n}?p)$$

Title compds. I [R = substituted Ph, wherein the substituent is selected AB from T or substituted pyridyl; R1 = (cyclo)alkyl, (cyclo)alkenyl, alkynyl; R2-4 = H, (cyclo)alkyl, (cyclo)alkenyl, oxo, representing two of the groups R2-4; X = S(0)0-2; n = 2; p = sum of non-H substituents <math>R2-4; T =alk(en/yn)yl, alkoxy, NO2, CN, halo; t = 1-5, provided that when T =alk(en/yn)yl, alkoxy, T is optionally substituted; G = halo, alkoxy, (cyclo) alk(en) yl, aryl, CN; g = 0-4, with the exception of halogen, which may be employed up to the perhalo level provided that when substituent G is alkyl, alkenyl, etc. then G is optionally substituted; Q = of (halo)alkyl, cycloalkyl, alkoxy, alkenyl, cycloalkenyl, etc.; q = 0-4; with some provisions] were prepared E.g. 2-chloroethylammonium chloride was reacted with (2-methyl-4-nitrophenyl)isothiocyanate (CH2Cl2, Et3N) to give the thiazolidine which was alkylated with i-Bu bromide (DMF, Cs2CO3, 90°C) to give II. Most compds. of the invention at 200 nM caused at least 30% inhibition of progesterone while, e.g., II caused >80% inhibition at the same concentration I are useful in the treatment of luteal deficiency, osteoprosis, hirsutism, etc.

IT 285122-01-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug; preparation and use of, e.g., 2-arylimino-1,3-thiazolidines as progesterone receptor binding ligands)

IT 285122-01-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug; preparation and use of, e.g., 2-arylimino-1,3-thiazolidines as progesterone receptor binding ligands)

RN 285122-01-2 HCAPLUS

Benzenamine, 2-methyl-N-[(4S)-3-(2-methylpropyl)-4-phenyl-2-thiazolidinylidene]-4-nitro-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

● HCl

D	E7	בי	R	Τ.	F
Γ	டப		. 13		

Referenced Author (RAU)	Year VOL (RPY) (RVL) (RPG)	Referenced Work (RWK)	Referenced File
Ambartsumova	1997 33	475	Chemistry of Heteroc	
Anon	1943	1	JP 4315609	†
Anon	1967	1	FR 1510014	HCAPLUS
Anon	1967	1	FR 1510015	HCAPLUS
Anon	1968	1	FR 1516854	HCAPLUS
Anon	1969	1	GB 1140776	HCAPLUS
Anon	1969	1	JP 4421095	1
Anon	1971	1	DE 1963192	HCAPLUS
Anon	1972	1	FR 2117337	HCAPLUS
Anon	1974	1 ,	GB 1342232	HCAPLUS
Anon	1974	1	GB 1377265	HCAPLUS
Anon	1976	1	DE 2511731	HCAPLUS
Anon	1977	1	GB 1467385	HCAPLUS
Anon	1978	1	GB 1527807	HCAPLUS
Anon	1978	1	HU 171587	
Anon	1978	1	DE 2658138	HCAPLUS
Anon	1980	1	GB 1579782	HCAPLUS
Anon	1980	1	GB 1580554	HCAPLUS
Anon	1986	1	SU 1209688	HCAPLUS
Anon	1986	1	DE 3505432	HCAPLUS
Anon	1987	1	EP 0240680	HCAPLUS
Anon	1988	1	JP 63041471 A2	HCAPLUS
Anon	1989	1	EP 0318253	HCAPLUS
Anon	1989	1	WO 8904595	HCAPLUS .
Anon	1994	1	EP 0600489	HCAPLUS
Anon	1995	1	EP 0683160	HCAPLUS
Anon	1995	1	JP 07304759 A2	HCAPLUS
Anon	1995	1	JP 7304759	
Anon	1995		WO 9533717	HCAPLUS
Anon	1996	1	WO 9614842	HCAPLUS
Anon	1998 33	151	Advances in Medicina	
Argay .	1980 B36	363	Acta Cryst	HCAPLUS
Arya	1977 15B	133	Indian J Chem	HCAPLUS
Bacchetti	1957	1	US 2784196 A	HCAPLUS
Balko	1981	1	US 4289778 A	HCAPLUS
Baumann	1988	!	US 4788209 A	HCAPLUS

Behner	11974		J		HCAPLUS
Behner	1975	1	1		HCAPLUS
Burke, J	11999		185	Postgraduate medicin	
Cherbuliez			331	Helvetica Chimica Ac	
Chiou	-	10	577		HCAPLUS
Culik	1972	!	1		HCAPLUS
Duerr	11967	ļ.		US 3345257 A	1
Durr	11978	ļ		US 4079144 A	I
Durr	1979	!	!		HCAPLUS
Durr	11979	ļ.	ļ		HCAPLUS
Enders	11979	!	!		HCAPLUS
Felix	1989	!	!		HCAPLUS
Felix	1990	1	!		HCAPLUS
Felix	1990	!			HCAPLUS
Fisher	•	!	100	· ·	HCAPLUS
-	1989	!	129	Organic Chemical Nom	
Garber	•	1 40	I 1120	T .	HCAPLUS
Hahn, H			1139	Agriculture Chem Bio	
Hanefeld			1799	Arch Pharm (Weinheim	
Hanefeld			160	Arch Pharm (Weinheim	
Hanefeld	•	•	199	Arch Pharm (Weinheim	
Heeres			1254	•	HCAPLUS
Ignatova			354	Khim Geterotsikl Soe	
Ignatova		-	11621	Khim Geterotsikl Soe	•
Ignatova	•		1307	The Journal of Chemi	*
Ignatova	•	:	1333	The Journal of Chemi	•
Ippen	• —	!	1760		HCAPLUS
John, D	11964		769 135	Basic Principles of	
Kalman	11987		125	•	HCAPLUS
Lang	•	l	1		HCAPLUS
Lang	•		 		HCAPLUS
Lempert		1	1		HCAPLUS
Luckenbaugh	•	1	ı 1877	•	HCAPLUS
March, J	•	:	1011	Advanced Organic Che US 5463069 A	
Masumoto	•	1216	I 1838		HCAPLUS
Mehta, R		:	1030	-	MEDLINE HCAPLUS
Metzger		 	1		
Metzger	11972	! !	! !	US 3689499 A	HCAPLUS
Metzger	11972	! !	1	US 3770693 A	! !
Metzger	•	 9	 1572		 HCAPLUS
Metzger Mizrakh	11986			Polym Prepr The Journal of Chemi	
Mizrakh	11989			The Journal of Chemi	
Mizrakh	11989			The Journal of Chemi	
Mizrakh	11986		173		 HCAPLUS
Mizrakh	11988		•		HCAPLUS
Mizrakh	11992		11498		HCAPLUS
Mohsen	11984	-	11166	J Pharma Sci	LITCAL HOS
Morrison, R	11983	•	1627	Organic Chemistry	; I
Nathanson	1987	! 	02 / 		HCAPLUS
Nathanson	1990	i i	! 		HCAPLUS :
Nomura, R	1989	1122	12407		HCAPLUS
Noseworthy, J			A40	•	HCAPLUS
Okawara	•	•	1507	• • •	HCAPLUS
Olzenko-Piontkowa	1971		127	Org Prep Proc Int	1
Peresleni	1977		1346	Khim Geterotikl Soed	i
Peresleni	11977		1278	The Journal of Chemi	
Raddatz	11988	•	,		HCAPLUS
Raman ·	11978		177	Res Commun Chem Phat	•
1 MIIIMII	, 15,0	,	1 - 1 1	, Johannan Onem Ende	,

L70 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:331534 HCAPLUS

DN 135:122450

TI Synthesis and antimicrobial activity of some 4-thiazoline-containing 1,2,4-triazoles

AU Ciuqureanu, Constantin; Ciuqureanu, Maria; Murarescu, Elena Doina

CS Univ. "Al. I. Cuza", Iasi, Rom.

SO Revista de Chimie (Bucharest, Romania) (2001), 52(1-2), 5-10 CODEN: RCBUAU; ISSN: 0034-7752

PB SYSCOM 18 SRL

DT Journal

LA Romanian

OS CASREACT 135:122450

GI

AB Title compds. such as I were prepared by 2 methods. In vitro antibacterial tests were run.

IT 351339-91-8P 351339-94-1P 351339-97-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (preparation and antimicrobial activity of 4-thiazoline-containing 1,2,4-triazoles)

IT 351340-00-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antimicrobial activity of 4-thiazoline-containing 1,2,4-triazoles)

ΙT 351339-91-8P

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation and antimicrobial activity of 4-thiazoline-containing 1,2,4-triazoles)

RN 351339-91-8 HCAPLUS

CN Benzoic acid, 4-[[4-phenyl-3-(2-propenyl)-2(3H)-thiazolylidene]amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-CH=CH_2 & 0 \\ \hline \\ C-OMe \\ \hline \\ S \end{array}$$

ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN L70

2001:78374 HCAPLUS AN

DN 134:147596

TI2-Arylimino-2,3-dihydrothiazoles, processes for their preparation, and their use as somatostatin receptor ligands

Moinet, Christophe; Sackur, Carole; Thurieau, Christophe IN

Societe de Conseils de Recherches et d'Applications Scientifiques PA (S.C.R.A.S, Fr.

PCT Int. Appl., 428 pp. SO

CODEN: PIXXD2

DTPatent

LΑ French

FAN.	CNT ·	1																
	PAT	ENT 1	. O <i>l</i>					DATE		APPLICATION NO.						DATE		
ΡI	WO	20010	00742	24		 A1		2001	0201	WO 2000-FR2095								
		W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
								DM,		•					-		-	
			•		-	•		JP,										
			LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,
			SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VN,
			YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM				
		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,
			DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,
			CF,	CG,	CI,	CM,	GΑ,	GN,	G₩,	ML,	MR,	NE,	SN,	TD,	TG			
	FR	2796	643			A1		2001	0126		FR 1	999-	9496			1	9990	722
	CA	23829	940			AA		2001	0201		CA 2	000-	2382	940		2	0000	721
	BR	20000	0126	47		Α		2002	0409		BR 2	000-	1264	7		2	0000	721
	ΕP	12029	980			A1		2002	0508		EP 2	000-	9585	75		2	0000	721
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,
								RO,										
	JP	2003	5054	53		Т2		2003	0212		JP 2	001-	5125	09		2	0000	721
	ΝZ	5165	99			Α		2004	0130		NZ 2	000-	5165	99		2	0000	721

	US 6727269	B1	20040427	US 2002-31429	20020115
	NO 2002000314	Α	20020306	NO 2002-314	20020121
PR	AI FR 1999-9496	Α	19990722		
	WO 2000-FR2095	W	20000721		
os	MARPAT 134:147596				
GI					

$$R^{2}$$
 N
 N
 N
 R^{3}
 R^{4}

$$\begin{array}{c|c} & & & & \\ & & & & \\ N & & & & \\ N & & & \\ N & & & \\ N & & \\ N & & \\ N & & \\ N & & \\ \end{array}$$

AΒ The invention concerns novel 2-arylimino-2,3-dihydrothiazole derivs. I and their racemates, enantiomers, combinations, and salts [wherein R1 = (un) substituted, particularly amino-substituted alk(en/yn)yl, (hetero)aryl, aralkyl, cycloalkyl, etc.; R2 = (un)substituted carbocyclic or heterocyclic aryl; R3 = alkyl, adamantyl, (un)substituted (hetero)aryl or (hetero)aralkyl, (un)substituted carbamoyl; R4 = H, alkyl, (un) substituted (hetero) aralkyl, etc.]. Also disclosed are methods of their preparation and their use as medicines, in particular for treating a wide variety of pathol. conditions or diseases involving somatostatin receptors. In particular, these pathol. conditions include acromegaly, pituitary adenoma, endocrine gastroenteropancreatic tumors (including the carcinoid syndrome), and gastrointestinal bleeding. Examples include 6 detailed syntheses, a listing of over 2800 characterized invention compds., and various precursor prepns. For instance, 4-H2NC6H4CH2CH2NH2 was bound to Wang resin p-nitrophenylcarbonate (at the aliphatic amino group), and the resin-bound amine reacted sequentially with PhCH2CH2NCS, bromopyruvic acid, and $4 ext{-ClC6H4CH2NH2} \cdot ext{to give, after acidic cleavage,}$ (Z)-isomeric title compound II. Ten selected compds. I inhibited binding of [125I-Tyr11] SRIF-14 to human somatostatin receptors in vitro with Ki < 200

IT 322740-74-9P 322740-76-1P 322740-77-2P 322740-78-3P 322740-79-4P 322740-80-7P 322741-53-7P 322741-54-8P 322741-55-9P 322741-56-0P 322741-57-1P 322741-58-2P 322741-62-8P 322741-63-9P 322741-64-0P 322741-65-1P 322741-66-2P 322741-67-3P

322742-25-6P 322742-26-7P 322742-27-8P 322742-28-9P 322742-29-0P 322742-30-3P

322742-31-4P 322743-27-1P 322743-28-2P.

322743-29-3P 322743-30-6P 322743-31-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of (arylimino)dihydrothiazoles as somatostatin receptor ligands)

IT 322740-74-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of (arylimino)dihydrothiazoles as somatostatin receptor ligands)

RN 322740-74-9 HCAPLUS

Benzeneethanamine, 4-[[3-(2-methylpropyl)-4-phenyl-2(3H)-thiazolylidene]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{i-Bu} & \text{CH}_2\text{-CH}_2\text{-NH}_2 \\ \text{Ph} & \text{N} & \text{CH}_2\text{-CH}_2\text{-NH}_2 \\ \end{array}$$

RETABLE

CN

Referenced Author	•	-	•	Referenced Work	Referenced
(RAU)			(RPG) 		File
Beilstein Institut Fuer Beilstein Institut Fuer	1978	126			
Beilstein Institut Fuer	•	i	' 	DATABASE CROSSFIRE	
Beilstein Institut Fuer	•	i	i İ	DATABASE CROSSFIRE	
Beilstein Institut Fuer	:	ĺ	ĺ	DATABASE CROSSFIRE	
Beilstein Institut Fuer	:1	1		DATABASE CROSSFIRE	
Beilstein Institut Fuer	:1	I		DATABASE CROSSFIRE	
Beilstein Institut Fuer	:	1		DATABASE CROSSFIRE	
Beilstein Institut Fuer	:	1	l	DATABASE CROSSFIRE	
Beilstein Institut Fuer		1	•	DATABASE CROSSFIRE	
Beilstein Institut Fuer					
Beilstein Institut Fuer					
Beilstein Institut Fuer	1984	21	1377	J HETEROCYCL CHEM	
Beilstein Institut Fuer	1931	18	147	J INDIAN CHEM SOC	
Beilstein Institut Fuer	1913	87	44	J PRAKT CHEM	
Beilstein Institut Fuer	1984	58	447	POL J CHEM	
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Beilstein Institut Fuer		•	45	UNIV KANS SCI BULL	
Duerr, D	11967			US 3345257 A	
Hassan, H	1998	•	863	CHEMICAL & PHARMACEU	
Hoechst Aktiengesellsch			l		HCAPLUS
Hoechst Aktiengesellsch	1 1982		l	, =	HCAPLUS
Kalcheva, V	1993	•	1319		
Lang, H	1982		l	• • • • • • • • • • • • • • • • • • • •	HCAPLUS
Liu, S	1998	-	•	JOURNAL OF MEDICINAL	
Omar, A	1984			JOURNAL OF PHARMACEU	
Sumitomo Chemical Compa	11995	l	ļ.	EP 0683160 A	HCAPLUS

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ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
L70
     2000:493535 HCAPLUS
AN
DN
     133:120323
ΤI
     Preparation of 2-aryliminothiazolidines and related compds. progesterone
    receptor binding agents
IN
     Dixon, Brian R.; Bagi, Cedo M.; Brennan, Catherine R.; Brittelli, David
     R.; Bullock, William H.; Chen, Jinshan; Collibee, William L.; Dally,
     Robert; Johnson, Jeffrey S.; Kluender, Harold C. E.; Lathrop, William F.;
     Liu, Peiying; Mase, Carol Ann; Redman, Aniko M.; Scott, William J.;
     Urbahns, Klaus; Wolanin, John J.
     Bayer Corporation, USA
PΑ
     PCT Int. Appl., 274 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
                                            ______
                         ____
     WO 2000042031
                          A2
                                20000720
                                            WO 1999-US29601
                                                                    19991214
PΙ
     WO 2000042031
                          A3
                                20001109
         W:
            AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
             SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2359562
                          AΑ
                                20000720
                                            CA 1999-2359562
                                                                    19991214
                                20011017
                                            EP 1999-968883
     EP 1144396
                          A2
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     BR 9916999
                                            BR 1999-16999
                                20011030
                                                                    19991214
                          Α
                                            TR 2001-200102041
     TR 200102041
                          T2
                                20011221
                                                                    19991214
                                            JP 2000-593599
     JP 2002534517
                          Т2
                                20021015
                                                                    19991214
                                            ZA 2001-5253
     ZA 2001005253
                          Α
                                20020905
                                                                    20010626
     NO 2001003318
                          Α
                                20010830
                                            NO 2001-3318
                                                                    20010704
                                            BG 2001-105761
     BG 105761
                          Α
                                20020329
                                                                    20010801
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19990114

19991214

Α

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PRAI US 1999-231906

WO 1999-US29601

MARPAT 133:120323

AB Title compds. (I; T = alkyl, alkoxy, aryl, CO2H, alkenyl, alkynyl, CHO, OH, NO2, cyano, halo, OCF3, etc.; R = aryl, heteroaryl; R1 = alkyl, cycloalkyl, heterocycloalkyl, alkenyl, cycloalkenyl, alkynyl; R2-R4 = H, alkyl, cycloalkyl, alkenyl, cycloalkenyl, aryl, heteroaryl, halo, O, etc.; X = O, S, SO, SO2; G = halo, OH, O, alkyl, alkenyl, cycloalkyl,

heterocycloalkyl, cycloalkenyl, aryl, heteroaryl, etc.; m=1-5; p, q=0-4; Z=CnH2n-r; n=2-5; r=sum of non-H substituents R2, R3, R4; with provisos), were prepared Thus, title compound (II), prepared from 2-chloroethylammonium chloride, 2-methyl-4-nitrophenyl isothiocyanate, and iso-Bu bromide, at 200 nM gave 80-100% inhibition of 3H-progesterone to the progesterone receptor.

IT 285122-01-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-aryliminothiazolidines and related compds. progesterone receptor binding agents)

IT 285122-01-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-aryliminothiazolidines and related compds. progesterone receptor binding agents)

RN 285122-01-2 HCAPLUS

CN Benzenamine, 2-methyl-N-[(4S)-3-(2-methylpropyl)-4-phenyl-2-thiazolidinylidene]-4-nitro-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

● HCl

L70 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:243751 HCAPLUS

DN 133:30351

TI Iminium salts in solid-state syntheses giving 100% yield

AU Kaupp, Gerd; Schmeyers, Jens; Boy, Juergen

CS Universitaet, Organic Chemistry I, Oldenburg, Germany

SO Journal fuer Praktische Chemie (Weinheim, Germany) (2000), 342(3), 269-280 CODEN: JPCHF4; ISSN: 1436-9966

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

OS CASREACT 133:30351

Numerous reaction types in the field of iminium salts are performed in the gas-solid and solid-solid techniques in order to reach 100% yield. The stoichiometric runs are waste-free and do not require costly workup. Frequently, iminium salts were avoided, as acid catalysis was dispensable. Thioureas and α -halogenated ketones give a variety of 2-aminothiazoles via thiuronium salts in quant. yield. A new intramol. solid-state thermal condensation is reported. Enamino ketones are synthesized quant. from anilines and 1,3-diketones without catalysis and

those can be used for quant. solid-state 4-cascade reactions. Solid paraformaldehyde is used to produce methylene imines and internally trapped methylene iminium salts. Benzoylhydrazones are produced again without catalysis in the solid state. Vacuum and ball-mill techniques are particularly useful in the production of highly sensitive iminium salts. Hexahydro-1,3,5-triazines cyclorevert upon exposure to HCl gas to give solid arylmethylene iminium chlorides as new versatile reagents. These are used in arylaminomethylations of β -naphthol and of themselves to give Troeger's bases in 3-cascades. More direct are 4-cascade Troeger's base syntheses by dissolving hexahydro-1,3,5-triaryltriazines in trifluoroacetic acid. Alkylations of imines with trimethyloxonium tetrafluoroborate and triphenylmethyl cation give highly sensitive quaternary iminium salts in the ball-mill. The products are characterized by spectroscopic techniques and d. functional theory (DFT) calcns. at the B3LYP 6-31G* level. Mol. movements in the crystal and surface passivation are investigated with atomic force microscopy (AFM) techniques.

IT 273933-52-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (solid-state synthesis and reactions of iminium salts)

IT 273933-52-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (solid-state synthesis and reactions of iminium salts)

RN 273933-52-1 HCAPLUS

CN Benzenamine, 4-chloro-N-(3-methyl-4-phenyl-2(3H)-thiazolylidene)-, monohydrobromide (9CI) (CA INDEX NAME)

HBr

RE	ומיז	ST.E.

(RAU)	(RPY) (RVL)	(RPG)	Referenced Work
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Ebara, N	1961 34	1151	Bull Chem Soc Jpn HCAPLUS
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Hanley 10/047,251

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                       |1973 |46
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                                         |Bull Chem Soc Jpn
                                                               HCAPLUS
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- L70 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
- AN 1998:377388 HCAPLUS
- DN 129:122609
- TI Synthesis of some new benzimidazoles bearing different heterocyclic moieties. Part III

andre of the state
4

- AU Mahmoud, A. M.; El-Ezbawy, S. R.; El-Sherief, H. A. H.; Sarhan, Abd El-Wareth A. O.
- CS Chem. Dep., Assiut Univ. Faculty Science, Assiut, 71516, Egypt
- SO Revue Roumaine de Chimie (1997), 42(12), 1155-1163 CODEN: RRCHAX; ISSN: 0035-3930
- PB Editura Academiei Romane
- DT Journal
- LA English
- AB Interaction of 2-(p-aminophenyl)benzimidazole (I) with chloroacetyl chloride afforded the N-chloroacetyl derivative II, which was also obtained from the cycloaddn. reaction of chloroacetyl chloride to Schiff bases. Reaction of II with mercaptans and/or secondary amines is reported. Condensation of I with aromatic aldehydes afforded Schiff bases, which on cyclocondensation with mercaptoacetic acid gave 4-thiazolidinones. Reaction of I with substituted isothiocyanates furnished thiourea derivs., which condensed with chloroacetic acid or its ester to form thiazolidinones.
- IT 210222-40-5P
 - RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 - (preparation and antibacterial activity of benzimidazoles)
- IT 210222-42-7P 210222-44-9P
 - RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and antibacterial activity of benzimidazoles)

IT 210222-40-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antibacterial activity of benzimidazoles)

RN 210222-40-5 · HCAPLUS

CN Benzenamine, 4-(1H-benzimidazol-2-yl)-N-(3-methyl-4-phenyl-2(3H)-thiazolylidene)- (9CI) (CA INDEX NAME)

RETABLE

Referenced Author (RAU)	Year (RPY)	•	PG (RPG)	Referenced Work (RWK)	Referenced File
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Mahmoud, A	1981	16	383	Eur J Med Chem	HCAPLUS
Mayer, R	1941	1	3	Rev Medical France	HCAPLUS
Mehta, K	1978	166	836	Ind J Chem	
Mehta, K	1978	50	81	J Inst Chem India	HCAPLUS
Merchant, J	1980		791	Chemistry and Indust	HCAPLUS
Nicholass, E	1928	18.6	1767	Compt Rend	1
Patel, P	1973	50	287	J Indian Chem Soc	HCAPLUS
Preston, P	1974	174	279	Chem Rev	HCAPLUS
Wilson, J	1983	136	2317	Aust J Chem	HCAPLUS
Yan, S	1978	15	297	J Heterocyclic Chem	HCAPLUS

L70 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

'AN 1993:448840 HCAPLUS

DN 119:48840

TI Electron impact mass spectrometry and metastable ion studies on some 2-(o-hydroxyphenyl-2(3H)-thiazoline-imine) and 1,3,4-thiadiazine derivatives

AU Hadjieva, P.; Kalcheva, V.; Tosheva, M.; Danieli, B.; Catinella, S.

CS Dep. Chem., Univ. Kliment Ochridsky, Sofia, 1126, Bulg.

SO Rapid Communications in Mass Spectrometry (1993), 7(3), 245-50 CODEN: RCMSEF; ISSN: 0951-4198

DT Journal

Ι

The electron-impact induced mass spectrometric behavior of nine 2-(o-hydroxyphenyl)-2(3H)imino-4-thiazolines (I; R1, R2, R3 given: Me, Me, H; Et, Me, H; Pr, Me, H; PhCH2, Me, H; PhCH2, Me, Cl; PhCH2, Me, NO2; Pr, Ph, H; Bu, Ph, H; NH2, Me, H) and 2-(o-hydroxyphenyl)imino-1,3,4-thiadiazine was studied in detail with the aid of accurate mass measurements, linked-scans for metastable-ion studies and deuterium-labeling expts. The related fragmentation pathways are strongly dependent on the presence of a substituent nitrogen atom in position 3, which can promote a hydrogen rearrangement process on the imine nitrogen and the further cleavage of the imine bond. In the case of an aryl substituent, specific fragmentation channels are activated, due to the high stability of the resultant product ions.

IT 148474-16-2 148474-17-3

RL: PRP (Properties)
 (mass spectrum of)

IT 148474-16-2

RL: PRP (Properties)
 (mass spectrum of)

RN 148474-16-2 HCAPLUS

CN Phenol, 2-[(4-phenyl-3-propyl-2(3H)-thiazolylidene)amino]- (9CI) (CA INDEX NAME)

L70 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1992:426475 HCAPLUS

DN 117:26475

TI Studies on synthesis of some quinazolinones bearing different heterocyclic moieties with expected biological activity

AU Hassan, H. Y.; Ismaiel, A. A.; El-Sherief, H. A. H.

CS Fac. Pharm., Assiut Univ., Assiut, Egypt

SO European Journal of Medicinal Chemistry (1991), 26(7), 743-8 CODEN: EJMCA5; ISSN: 0223-5234

DT Journal

LA English

GΙ

$$N$$
 N
 Me

AB Several antimicrobial quinazolinones I (R = NHC(S)NHR1, R1 = Me Et, Bu, CH2Ph, Bz, cyclohexyl; R = 3-alkyl-4-aryl-2,3-dihydrothiazol-2-ylideneamino, 3-alkyl-4-oxothiazolidin-2-ylideneamino) were prepared from I (R = NH2) by treatment with alkyl isocyanates followed by cyclocondensation with phenacyl bromides or ClCH2CO2H.

IT 138802-36-5P 138802-37-6P 138802-38-7P 138802-39-8P 138802-40-1P 138802-41-2P 138802-42-3P 138802-43-4P 138802-44-5P

Ι

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antimicrobial activity of)

IT- 138802-36-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antimicrobial activity of)

RN 138802-36-5 HCAPLUS

CN 4(3H)-Quinazolinone, 2-methyl-3-[4-[(3-methyl-4-phenyl-2(3H)-thiazolylidene)amino]phenyl]- (9CI) (CA INDEX NAME)

L70 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:77226 HCAPLUS

DN 112:77226

TI 5-Lipoxygenase-inhibiting 4-(4-phenyl-1-piperazinyl)phenols and their preparation and pharmaceutical compositions

IN Van Wauwe, Jean Pierre Frans; Heeres, Jan; Backx, Leo Jacobus Jozef

PA Janssen Pharmaceutica N. V., Belg.

SO Eur. Pat. Appl., 40 pp. CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE
PI EP 331232 A2 19890906 EP 1989-200424 19890221

		331232			A3	19910424				
	EP	331232		~	B1	19940518	an			
			BE,	CH,		ES, FR, GB,				
		1331757			A1	19940830		1989-58783		19890110
		4931444			Α	19900605		1989-29701	-	19890112
		02003678			A2	19900109	JP	1989-38486		19890220
		07005564			B4	19950125				
		105711			Ε	19940615		1989-20042	_	19890221
		2056190			Т3	19941001	ES	1989-20042	4	19890221
	ΑU	8930739			A1	19890831	AU	1989-30739		19890224
	ΑU	615519			B2	19911003				
	DK	8900918			Α	19890830	DK	1989-918		19890227
	FI	8900931			Α	19890830	FI	1989-931		19890227
	FI	97383			В	19960830				
	FI	97383	•		С	19961210				
	ИО	8900813			Α	19890830	ИО	1989-813		19890227
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	IL	89426			A1	19930610	$_{ m IL}$	1989-89426		19890227
	CN	1036569			Α	19891025	CN	1989-10093	1	19890228
	CN	1021223			В	19930616				
	HU	52080			A2	19900628	HU	1989-927		19890228
	ZA	8901547			Α	19901031	ZA	1989-1547		19890228
	RU	2107064			C1	19980320	RU	1989-46135	48	19890228
	KR	133074			В1	19980417	KR	1989-2435		19890228
	HU	68931			A2	19950828	HU	1993-3071		19931028
PRAI	US	1988-161	825		Α	19880229				
	ΕP	1989-200	424		Α	19890221				
	HU	1989-927			Α	19890228				•
os	MAI	RPAT 112:	7722	6						
GI										

Over 220 title compds. I [R1, R2 = H, halo, C1-6 alkyl; R3, R4 = H, halo, NH2, NO2, CF3; Y = H, NO2, NH2, mono- or dialkylamino, alkylcarbonylamino, C1-6 alkyl, alkylcarbonyl, OH, halo, mono- or dialkylaminosulfonyl, various (un)substituted 5- or 6-membered N-containing heterocycles with optional O or S atoms] and/or their acid addition salts and stereoisomers were prepared as selective inhibitors of 5-lipoxygenase. Thus, 4-[4-(4-methoxyphenyl)-1-piperazinyl]benzenamine was condensed with (MeO)2CHCH2NCS to give the thiourea (36%), followed by cyclization in HCO2H to give a dihydromethoxythiazolamine (52%), alkylation with EtBr and NaOH in DMF (44.4%) and demethylation/elimination using 48% HBr (81.5%) to give I [R1-R4 = H, Y = ethyl(2-thiazolyl)amino]. Various I gave up to 100% inhibition of 5-lipoxygenase in vitro at 2.5 mM and up to 94% inhibition of dextran-induced mouse-ear edema at 10 mg/kg orally. Capsules, tablets, oral and injectable solns., and other forms containing I

Ι

were prepared

IT 125234-74-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as lipoxygenase inhibitor)

IT 125234-74-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as lipoxygenase inhibitor)

RN 125234-74-4 HCAPLUS

CN Phenol, 4-[4-[4-[(3-ethyl-4-phenyl-2-thiazolidinylidene)amino]phenyl]-1piperazinyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

OH

L70 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1986:56408 HCAPLUS

DN 104:56408

TI Inclusion compound of N,N-dimethyl-2-chloro-5-[3-methyl-2-(phenylimino)-4-thiazolin-4-yl]phenylsulfonamide with hypolipemic properties

IN Seidel, Heinz Ruediger

PA Hoechst A.-G., Fed. Rep. Ger.

SO Ger. Offen., 7 pp.

CODEN: GWXXBX

DT Patent LA German FAN.CNT 1

T.VI	V. CIVI I				
	PATENT NO.	KIND DATE		APPLICATION NO.	DATE
ΡI	DE 3329517	A1	19850228	DE 1983-3329517	19830816
	EP 141076	Al	19850515	EP 1984-109377	19840808
	R: AT, BE, CH,	DE, FR	, GB, IT, LI	, LU, NL, SE	
	ES 535135	Al	19851116	ES 1984-535135	19840814
	DK 8403923	Α	19850217	DK 1984-3923	19840815
	AU 8431961	A1	19850221	AU 1984-31961	19840815
	ZA 8406327	A	19850327	ZA 1984-6327	19840815
	JP 60058969	A2	19850405	JP 1984-169454	19840815
PRA	AI DE 1983-3329517	Α	19830816		

AB The dissoln. rate and absorption of HCG 497 [N,N-dimethyl-2-chloro-5-[3-methyl-2-(phenylimino)-4-thiazolin-4-yl]phenylsulfonamide] are enhanced by complexing with β -cyclodextrin. Thus, 100 g β -cyclodextrin in 360 mL H2O was treated with 16.32 g HCG 497 and 48 mL 1N HCl to give the inclusion complex. HCG 497 showed a much higher dissoln. rate from capsules containing the complex, compared to capsules containing HCG 497 as such.

The complex can therefore be used in hypolipemic prepns.

IT 99941-82-9P

RL: PREP (Preparation)

(preparation of, as hypolipemic with enhanced dissoln. and absorption)

IT 99941-82-9P

RL: PREP (Preparation)

(preparation of, as hypolipemic with enhanced dissoln. and absorption)

RN 99941-82-9 HCAPLUS

CM 1

CRN 77989-60-7

CMF C18 H18 C1 N3 O2 S2

$$\begin{array}{c|c}
O & S - NMe_2 \\
N & C1 \\
S & S - NMe_2
\end{array}$$

CM 2

CRN 7585-39-9 CMF C42 H70 O35

Absolute stereochemistry.

ОН

ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN L70

1985:437403 HCAPLUS AN

103:37403 DN

Introduction of selenium to heterocyclic compounds. ΤĮ Part IV. of 2-imino-4-thiazoline derivatives

ΑU Korohoda, Maria Jolanta; Bojarska, Aleksandra Barbara

CS

Dep. Chem., Pedagog. Coll., Krakow, 30084, Pol. Polish Journal of Chemistry (1984), 58(4-5-6), 447-53 SO CODEN: PJCHDQ; ISSN: 0137-5083

Journal DT

LΑ English

CASREACT 103:37403 os

GΙ

AB The title compds. I (R = Me, Et, Ph, substituted Ph, R1 = Ph, substituted Ph) were prepared in 70.5-97.0% yields by cyclocondensation of BrCH2COPh with RNHCSNHR1. Methylation of I by Me2SO4 followed by reaction with NaHSe gave 38.5-85.0% thiazolines II (R = Me, Et, Ph, p-tolyl, p-MeOC6H4).

IT 97118-81-5P 97118-82-6P 97118-83-7P 97118-84-8P 97118-85-9P 97118-86-0P 97118-87-1P 97118-88-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and sequential methylation and reaction)

(preparation and sequential methylation and reaction with sodium hydrogen selenide)

IT 97118-81-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and sequential methylation and reaction with sodium hydrogen selenide)

RN 97118-81-5 HCAPLUS

CN Benzenamine, N-(3-methyl-4-phenyl-2(3H)-thiazolylidene)- (9CI) (CA INDEX NAME)

L70 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN .

AN 1983:72082 HCAPLUS

DN 98:72082

TI Thiazoline derivatives, their use and their pharmaceutical preparations

IN Lang, Hans Jochen; Seuring, Bernhard; Granzer, Ernold

PA Hoechst A.-G., Fed. Rep. Ger.

SO Eur. Pat. Appl., 45 pp.

CODEN: EPXXDW

DT Patent

LA German

FAN.CNT 1

LAM.	~IVT	T										
	PATENT NO.			KIND DATE		APPLICATION NO.		0.	DATE			
						-						
ΡI	EΡ	55458			A2		1982	0707	EP.	1981-11067	7	19811222
	ΕP	55458			A3		1982	1020				
	ΕP	55458			В1		1985	0213				
		R: AT	, BE,	CH,	DE,	FR	, GB,	IT,	LU, NI	L, SE		
	DE	3049460			A1		1982	0729	DE	1980-30494	60	19801230
	AT	11778			E		1985	0215	AT	1981-11067	7	19811222
	ES	508293			A1		1983	0401	ES	1981-50829	3	19811223
	FI	8104175			Α		1982	0701	FI	1981-4175		19811228
	JР	5713447	2		A2		1982	0819	JP	1981-21009	3	19811228
	US	4421757			Α		1983	1220	US	1981-33514	9	19811228
	IL	64653			A1		1985	0929	IL	1981-64653		19811228
	DK	8105811			Α		1982	0701	DK	1981-5811		19811229
	NO	8104468			Α		1982	0701	ИО	1981-4468		19811229
	NO	154551			В		1986	0707				
	ZA	8108968			A		1982	1124	ZA	1981-8968		19811229
		26885			0		1983	0928	HU	1981-3984		19811229

	HU	184976	В	19841128		
	CA	1173836	A1	19840904	CA 1981-393285 1	9811229
	ΑU	8179068	A1	19820708	AU 1981-79068 1	9811230
	ΑU	542670	B2	19850228		
	ES	518272	A1	19830901	ES 1982-518272 1	9821216
	ES	518273	A1	19830901	ES 1982-518273 1	9821216
	ES	518274	A1	19830901	ES 1982-518274 1	9821216
	ES	518271	A1	19840216	ES 1982-518271 1	9821216
PRAI	DE	1980-3049460	А	19801230		
	ΕP	1981-110677	А	19811222		
GI						

Ι

AB Thiazolines I (R = H, halo, Me; R1 = C1-3 alkyl; R2, R3 = H, halo, C1-4 alkyl or alkoxy; R4, R5 = H, C1-4 alkyl; N R4R5 = saturated ring with ≤6 members; R6 = H, C1-4 acyl), useful in lowering cholesterol in serum very low and low d. lipoproteins with little or no effect on high d. lipoproteins and thus useful in treating atherosclerosis, were prepared by 5 methods. MeNHCSNHC6H4OH-4 and COC12 in THF gave C1C(NHMe):NC6H4OH-4.HC1 which cyclized with 4,3-C1(Me2NSO)2C6H3COCH2SH in Me2CHOH by treating the mixture successively with NEt3 in a little Me2CHOH, CHC13 with overnight stirring, and AcOH to give II. Rats were treated with 10 mg/kg II per day orally for 7 days; this treatment lowered cholesterol in serum 9%, in the very low d. serum lipoprotein 54%, in low d. lipoprotein 17%, and in high d. serum lipoprotein 4%.

IT 84386-25-4

RL: PROC (Process)
(acidification of)

IT 84386-62-9P 84386-80-1P 84387-57-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and alkalinization of)

IT 84386-25-4P 84386-40-3P 84386-47-0P

84387-52-0P

RL: SPN (Synthetic preparation); PREP (Preparation).

(preparation and selective cholesterol lowering in very low and low d. serum lipoproteins)

IT 84271-98-7P 84386-17-4P 84386-23-2P

84386-24-3P 84386-26-5P 84386-27-6P

84386-28-7P 84386-29-8P 84386-30-1P

84386-31-2P 84386-32-3P 84386-33-4P

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84386-34-5P 84386-35-6P 84386-36-7P
     84386-37-8P 84386-38-9P 84386-39-0P
     84386-41-4P 84386-42-5P 84386-43-6P
     84386-44-7P 84386-45-8P 84386-46-9P
     84386-48-1P 84386-49-2P 84386-50-5P
     84386-51-6P 84386-52-7P 84386-53-8P
     84386-54-9P 84386-55-0P 84386-56-1P
     84386-57-2P 84386-58-3P 84386-59-4P
     84386-60-7P 84386-61-8P 84386-63-0P
     84386-64-1P 84386-65-2P 84386-66-3P
     84386-67-4P 84386-68-5P 84386-69-6P
     84386-70-9P 84386-71-0P 84386-72-1P
     84386-73-2P 84386-74-3P 84386-75-4P
     84386-76-5P 84386-77-6P 84386-78-7P
     84386-79-8P 84386-81-2P 84386-82-3P
     84386-83-4P 84386-84-5P 84386-85-6P
     84386-86-7P 84386-87-8P 84386-88-9P
     84386-89-0P 84386-90-3P 84386-91-4P
     84386-92-5P 84386-93-6P 84386-94-7P
     84386-95-8P 84386-96-9P 84386-97-0P
     84386-98-1P 84386-99-2P 84387-50-8P
     84387-51-9P 84387-53-1P 84387-54-2P
     84387-55-3P 84387-56-4P 84387-59-7P
     84393-67-9P 84393-68-0P 84405-60-7P
     84405-61-8P 84405-62-9P 84405-63-0P
     84405-64-1P 84405-65-2P 84405-66-3P
     84405-67-4P 84405-68-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
IT
     84386-19-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation, acylation of, and cholesterol lowering in very low and low d.
        serum lipoproteins)
ΙT
     84387-49-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation, saponification of, and selective cholesterol lowering in very
low and
        low d. serum lipoproteins)
TΤ
     84386-25-4
     RL: PROC (Process)
        (acidification of)
RN
     84386-25-4 HCAPLUS
     Benzenesulfonamide, 2-chloro-5-[2,3-dihydro-2-[(4-hydroxyphenyl)imino]-3-
CN
     methyl-4-thiazolyl]-N-methyl- (9CI) (CA INDEX NAME)
```

1981:425048 HCAPLUS ΑN

DN 95:25048

TI Thiazolidine derivatives or their pharmacologically compatible acid addition salts

Lang, Hans Jochen; Seuring, Bernhard; Granzer, Ernold IN

PA Hoechst A.-G., Fed. Rep. Ger.

Ger. Offen., 110 pp. SO

CODEN: GWXXBX

DTPatent

LA German

GΙ

FAN.	CNT	1								
	PA'	TENT NO.		KINI)	DATE	Α	PPLICATION NO.	Γ	DATE
					-		_		, -	
ΡI	DE					19810115		E 1979-2926771		19790703
				A1		19810216		S 1980-492847		19800627
		492871				19810216	E	S 1980-492871	1	19800627
		492872		A1		19810216	E	S 1980-492872	1	L9800627
		492873		A1		19810216		S 1980-492873	-	19800627
	ES	492874		A1		19810216		5 1980-492874		19800627
		23964		A1		19810218	Ε	P 1980-103688	1	19800628
	ΕP	23964		В1		19830216				
		R: AT, BE,	CH,	-			NL,	SE		
		2524		E				г 1980-103688	1	19800628
		8002094		Α		19810104		I 1980-2094		L9800701
				Α				S 1980-165218		19800701
				Α				K 1980-2865	_	19800702
		8001995		Α			N	0 1980-1995	1	19800702
				В		19860414				
		8060037		A1		19810115		J 1980-60037	1	L9800702
						19831201				
		8003979		Α		19810624		4 1980-3979	_	L9800702
		24426		O B		19830228		J 1980-1643	1	19800702
								•		
						19831101		A 1980-355222		L9800702
		60468		A1		19841130		L 1980-60468		L9800702
		70114				19841130		L 1980-70114		L9800702
		56010180				19810202		P 1980-91605		19800703
		8404120		Α		19810105	N	0 1984-4120	1	L9841016
PRAI		1979-2926771		Α		19790703				
		1980-103688		Α		19800628				
	ΙL	1980-60468		A3		19800702			•	

$$\begin{array}{c|c}
R^5 \\
\hline
R_1 \\
R_2
\end{array}$$

$$\begin{array}{c|c}
R^4 \\
R^3 \\
\end{array}$$

Anticholesteremic (no data) thiazolines I (R = H, halogen, alkyl; R1 = AΒ alkyl, cycloalkyl, alkenyl; R2-R4 = H, halogen, alkyl, alkoxy, OCH2O, OCH2CH2O, NMe2, NEt2, CF3; R5, R6 = H, alkyl; R7 = H, alkyl, cycloalkyl, allyl, CH2CH2Ph, optionally substituted CH2Ph; NR6R7 = heterocyclic) were

Ι

```
prepared Thus, cyclocondensation of 4,3-Cl(Me2NSO2)C6H3COCH2Br with
     PhNHCSNHMe gave a thiazolidinol whose dehydration with acid gave I (R =
     C1, R1 = R6 = R7 = Me, R2-R5 = H).
TΤ
     77990-93-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and amination of)
IT
     77989-59-4P 77989-60-7P 77989-61-8P
     77989-62-9P 77989-63-0P 77989-64-1P
     77989-65-2P 77989-66-3P 77989-67-4P
     77989-68-5P 77989-69-6P 77989-70-9P
     77989-71-0P 77989-72-1P 77989-73-2P
     77989-74-3P 77989-75-4P 77989-76-5P
     77989-77-6P 77989-78-7P 77989-79-8P
     77989-80-1P 77989-81-2P 77989-82-3P
     77989-83-4P 77989-84-5P 77989-85-6P
     77989-86-7P 77989-90-3P 77989-91-4P
     77989-92-5P 77989-93-6P 77989-94-7P
     77989-95-8P 77989-98-1P 77989-99-2P
     77990-00-2P 77990-01-3P 77990-04-6P
     77990-05-7P 77990-06-8P 77990-07-9P
     77990-08-0P 77990-09-1P 77990-10-4P
     77990-11-5P 77990-12-6P 77990-13-7P
     77990-14-8P 77990-15-9P 77990-16-0P
     77990-17-1P 77990-18-2P 77990-19-3P
     77990-20-6P 77990-21-7P 77990-22-8P
     77990-23-9P 77990-25-1P 77990-26-2P
     77990-29-5P 77990-30-8P 77990-31-9P
     77990-32-0P 77990-33-1P 77990-34-2P
     77990-35-3P 77990-36-4P 77990-37-5P
     77990-38-6P 77990-39-7P 77990-40-0P
     77990-41-1P 77990-42-2P 77990-43-3P
     77990-44-4P 77990-45-5P 77990-46-6P
     77990-47-7P 77990-48-8P 77990-49-9P
     77990-50-2P 77990-51-3P 77990-52-4P
     77990-53-5P 77990-54-6P 77990-55-7P
     77990-56-8P 77990-57-9P 77990-58-0P
     77990-59-1P 77990-60-4P 77990-62-6P
     77990-63-7P 77990-64-8P 77990-65-9P
     77990-66-0P 77990-67-1P 77990-68-2P
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     77990-74-0P 77990-75-1P 77990-76-2P
     77990-77-3P 77990-78-4P 77990-79-5P
     77990-80-8P 77990-81-9P 77990-83-1P
     77990-84-2P 77990-85-3P 77990-86-4P
     77990-87-5P 77990-88-6P 77990-89-7P
     77990-90-0P 77990-91-1P 77990-92-2P
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     78006-63-0P 78006-64-1P 78006-65-2P
     78006-67-4P 78006-68-5P 78006-69-6P
     78020-29-8P 78134-35-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
IT
     77990-93-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and amination of)
RN
     77990-93-3 HCAPLUS
     Benzenesulfonyl chloride, 2-chloro-5-[2,3-dihydro-3-methyl-2-(phenylimino)-
CN
```

$$\begin{array}{c|c} Me & \\ \\ N & \\ O = S - C1 \\ \\ O & \\ \end{array}$$

● HBr

L70 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1979:87338 HCAPLUS

DN 90:87338

TI Studies on heterocyclic cation systems. Part XII. Reactions of 2-dialkylamino-5-phenyl-1,3-oxathiolium cation with nucleophiles containing an amino group

AU Hirai, Kentaro; Ishiba, Teruyuki

CS Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, Japan

SO Chemical & Pharmaceutical Bulletin (1978), 26(10), 3017-22 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

OS CASREACT 90:87338

GI For diagram(s), see printed CA Issue.

AB Reactions of 2-dialkylamino-1,3-oxathioliums (I) (NR2 = piperidino, morpholino, NMe2; X = ClO4, HSO4) with amino-nucleophiles provide simple access to a variety of heterocyclic compds. Thiadiazines and thiazoles were readily obtained from the reaction with hydrazines and NH3, resp. The intermediates, which were easily converted into thiazoles, were also isolated. Reaction of I with aromatic amines gave ring-opened ketones and 2-arylimino-1,3-oxathioles, depending upon the reaction conditions. Reactions of I with aromatic and aliphatic amines in boiling HOAc gave 2-iminothiazoline derivs.

IT 68981-15-7P

IT 68981-15-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 68981-15-7 HCAPLUS

CN Benzenamine, N-(4-phenyl-3-propyl-2(3H)-thiazolylidene)-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

L70 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1979:22879 HCAPLUS

DN 90:22879

Synthesis and antiinflammatory activity of 2-amino- and 2-alkylamino-6-benzothiazoleacetic acids, 4-(2'-benzothiazolylamino)-, 4-(4'-substituted-2-thiazolylamino)- and $4-(4'-substituted-3'-alkyl-\Delta4'-thiazoline-2'-imino)phenylacetic acids$

AU Sawhney, S. N.; Arora, S. K.; Singh, J. V.; Bansal, O. P.; Singh, S. P.

CS Dep. Chem., Kurukshetra Univ., Kurukshetra, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1978), 16B(7), 605-9 CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

OS CASREACT 90:22879

GΙ

HO2CCH2

S
NHR

I
R1

II

$$R^4$$

S
NH

CH2CO2H

III

 R^4

S
NH

CH2CO2H

III

 R^4

III

Thiazoles and benzothiazoles containing the CH2CO2H moiety were prepared and some were tested for antiinflammatory activity. The compds. are I (R = H, Me, Et, Pr, Bu), II (R1 = Me, Ph or substituted phenyl), III (R2 = Me, Et; R3 = Ph or substituted phenyl), and IV (R4 = H, Me, MeO, Cl, Br, NO2). E.g., I and III were prepared by thiocyanation of p-H2NC6H4CH2CO2H to give phenylthioureas, which underwent cyclization in the presence of Br or cyclocondensation with R3COCH2Br. III (R2 = Et, R1 = p-tolyl) showed a

```
38.2% inhibition of carrageenin-induced edema in the rat at 120 mg/kg.
IT
     68194-87-6P 68194-95-6P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (preparation and antiinflammatory activity of)
IT
     68194-88-7P 68194-89-8P 68194-90-1P
     68194-91-2P 68194-92-3P 68194-93-4P
     68194-94-5P 68195-04-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
IT
     68194-87-6P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (preparation and antiinflammatory activity of)
RN
     68194-87-6 HCAPLUS
     Benzeneacetic acid, 4-[(3-methyl-4-phenyl-2(3H)-thiazolylidene)amino]-
CN
           (CA INDEX NAME)
```

=> d his

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(FILE 'HOME' ENTERED AT 07:43:08 ON 27 APR 2005)
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FILE 'HCAPLUS' ENTERED AT 07:43:15 ON 27 APR 2005
           3025 S THOMAS C?/AU
L1
                E WINDSOR J/AU
L2
             13 S E3 OR E5 OR E6 OR E9
L3
            356 S ROUX S?/AU
            655 S LLOYD A?/AU
L4
            523 S HURLEY L?/AU
L5
L6
           4538 S L1-L5
L7
              7 S L6 AND ABC (5A) TRANSPORTER?
L8
              7 S L6 AND ECTO(A) PHOSPHATASE?
L9
              9 S L7 OR L8
                 SELECT L9 RN 1-9
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FILE 'REGISTRY' ENTERED AT 07:47:48 ON 27 APR 2005
L10
             66 S E1-E66
L11
                STR
L12
              0 S L11
              0 S L11 FUL
L13
L14
                STR L11
             33 S L14
L15
           3856 S L14 FUL
L16
              0 S L10 AND L16
L17
                 STR L14
L18
```

```
L19
             33 S L18
L20
           3873 S L18 FUL
L21
                STR
                SAVE TEMP L18 HAN251STR/O
               SAVE TEMP L20 HAN251FUL/A
              0 S L21 SUB=L20 SAM
L22
              0 S L21 FUL SUB=L20
L23
L24
              STR L21
L25
             0 S L24
L26
              0 S L24 SUB=L20 SAM
               DELETE HAN251FUL/A
               DELETE HAN251STR/Q
L27
               STR
L28
               STR L27
               SCREEN 1840
L29
L30
             50 S L28 AND L29
L31
        101049 S L28 AND L29 FUL
L32
                STR
L33
                STR L32
                SAVE TEMP L31 HAN251STR/Q
                SAVE TEMP L28 HAN251STR/Q
                SAVE TEMP L31 HAN251FUL/A
L34
              0 S L33 SAM SUB=L31
L35
               STR L33
              1 S L35 FUL SUB=L31
L36
               SAVE TEMP L36 HAN251SUB1/A
L37
               STR
L38
            50 S L37 SAM SUB=L31
L39
          4988 S L37 FUL SUB=L31
                SAVE TEMP HAN251SUB2/Q L37
                SAVE TEMP L39 HAN251FUL1A/A
                STR
L40
            11 S L40 CSS SAM SUB=L39
           119 S L40 CSS FUL SUB=L39
                STR L40
L43 .
           4619 S L43 CSS FUL SUB=L39
     FILE 'HCAPLUS' ENTERED AT 10:55:59 ON 27 APR 2005
             7 S L44 AND L6
L45
             23 S. L44 AND P/DT
L46
     FILE 'REGISTRY' ENTERED AT 10:58:13 ON 27 APR 2005
L47
         20779 S ?PHOSPHATASE?/CNS
     FILE 'HCAPLUS' ENTERED AT 11:01:31 ON 27 APR 2005
L48
              7 S L44 AND (L47 OR ?PHOSPHATASE?)
                E A/RL
L49
             8 S L44 (L) AGRICULTURAL USE/RL
             13 S L44 AND (AGR? OR PLANT?)/SC, SX, CT, CW, BI
L50
             8 S L44 AND ?HERBICID?
L51
L52
             8 S L44 AND ?INSECTICID?
L53
             1 S L44 AND ?PARASIT?
             3 S L44 AND WEED?
L54
             4 S L44 AND PESTICID?
L55
              3 S L44 AND (PEA# OR CARROT# OR FLOWER# OR RICE# OR WHEAT?)
L56
               E DRUG RESISTANCE/CT
               E DRUG RESISTANCE/CT
               E DRUG RESISTANCE/CT
L57
              4 S E3+OLD, NT, PFT, RT AND L44
```

L58		E TRANSPORT PROTEINS/CT 6 S TRANSPORT PROTEINS/CT (L)ABC AND L44
	FILE	'REGISTRY' ENTERED AT 11:16:01 ON 27 APR 2005
L59	FILE	'HCAPLUS' ENTERED AT 11:16:22 ON 27 APR 2005 7 S L36
L60	FILE	'CAOLD' ENTERED AT 11:25:01 ON 27 APR 2005 1 S L44 SELECT AN EDIT /AN /OREF
L61 L62 L63 L64 L65 L66 L67 L68 L69 L70	FILE	'HCAPLUS' ENTERED AT 11:30:34 ON 27 APR 2005 2 S E1 SELECT AN L61 1 1 S E2-E3 31 S L44 1 S L62 AND L63 15 S L45 OR L48-L59 8 S L65 AND P/DT NOT L6 1 S L62 AND L66 7 S L66 NOT L67 7 S L65 NOT L66-L68 16 S L63 NOT L64-L69

FILE 'HCAPLUS' ENTERED AT 12:06:15 ON 27 APR 2005

FILE 'CAOLD' ENTERED AT 12:07:23 ON 27 APR 2005

FILE 'HCAPLUS' ENTERED AT 12:08:03 ON 27 APR 2005



STIC Search Report Biotech-Chem Library

STIC Database Tracking Number 1977/C

TO: Susan Hanley

Location: rem/3d70/3e71

Art Unit: 1651

Tuesday, April 26, 2005

Case Serial Number: 10/047251

From: Mary Jane Ruhl

Location: Biotech-Chem Library

Remsen 1-A-62

Phone: 571-272-2524

maryjane.ruhl@uspto.gov

Search Notes

Examiner Hanley,

Here are the results for your recent search request.

Please feel free to contact me if you have any questions about these results.

Thank you for using STIC services. We appreciate the opportunity to serve you.

Sincerely,

Mary Jane Ruhl Technical Information Specialist STIC Remsen 1-A-62 Ext. 22524



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=> d his ful
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FILE 'HCAPLUS' ENTERED AT 10:38:17 ON 26 APR 2005
                E THOMAS COLLIN E/AU
              5 SEA ABB=ON ("THOMAS COLLIN E"/AU OR "THOMAS COLLIN ERNEST"/AU
L5
                OR "THOMAS COLLIN R"/AU)
                E WINDSOR J BRIAN/AU
             10 SEA ABB=ON ("WINDSOR J B"/AU OR "WINDSOR J BRIAN"/AU)
L6
                E ROUX STAN J/AU
             90 SEA ABB=ON ("ROUX STAN J"/AU OR "ROUX STANLEY"/AU OR "ROUX
1.7
                STANLEY J"/AU OR "ROUX STANLEY J JR"/AU)
                E LLOYD ALAN M/AU
             25 SEA ABB=ON ("LLOYD ALAN M"/AU OR "LLOYD ALAN MARTIN"/AU)
L8
                E HURLEY LAURENCE/AU
L9
            214 SEA ABB=ON ("HURLEY LAURENCE"/AU OR "HURLEY LAURENCE H"/AU OR
                "HURLEY LAURENCE HAROLD"/AU)
              1 SEA ABB=ON L5 AND L6 AND L7 AND L8 AND L9
L10
                SELECT RN L10 1-1
     FILE 'REGISTRY' ENTERED AT 10:40:04 ON 26 APR 2005
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L11
                OR 168832-50-6/BI OR 171248-07-0/BI OR 291536-79-3/BI OR
                291536-80-6/BI OR 291536-81-7/BI OR 291536-82-8/BI OR 291536-83
                -9/BI OR 291536-84-0/BI OR 291536-85-1/BI OR 291536-86-2/BI OR
                291536-87-3/BI OR 291536-88-4/BI OR 291536-89-5/BI OR 291536-90
                -8/BI OR 291536-91-9/BI OR 291536-92-0/BI OR 41481-51-0/BI OR
                50-81-7/BI OR 56-65-5/BI OR 9013-05-2/BI)
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L12
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L13
               ANALYZE L12 1-1 CT : 15 TERMS
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L14.
               STR
L15
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L16
              0 SEA SSS FUL L14
L17
               STR L14
             4 SEA SSS FUL L18 4 complete from Reg. for Str. IX
L18
L19
L20
     FILE 'HCAPLUS' ENTERED AT 11:38:47 ON 26 APR 2005
L21
            10 SEA ABB=ON L20
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L22
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L23
              0 SEA SSS SAM L22
L24
              0 SEA SSS FUL L22
L25
               STR L22
              0 SEA SSS SAM L25
L26
L27
              0 SEA SSS FUL L25
L28
               STR L25
L29
              0 SEA SSS SAM L28
               STR L28
L30
           128 SEA SSS FUL L30 128 compde from Rey for Str. XVI
L31
L32
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FILE 'HCAPLUS' ENTERED AT 11:55:09 ON 26 APR 2005

L33 L34	11 SEA ABB=ON L32 14 SEA ABB=ON L21 OR L33
	FILE 'REGISTRY' ENTERED AT 11:55:44 ON 26 APR 2005
	E PHOSPHATASE/CN
L35	1 SEA ABB=ON PHOSPHATASE/CN
	FILE 'HCAPLUS' ENTERED AT 11:56:17 ON 26 APR 2005
L36	7 SEA ABB=ON L34 AND ((L35 OR ?PHOSPHATAS?)(W)?INHIBIT? OR
	(?DRUG?(W)?RESIST?)(4A)(?DECREAS? OR ?INHIBIT? OR ?LESSEN? OR
	?PREVENT? OR ?CONTROL?) OR ?PEAS? OR ?CARROT? OR ?FLOWER? OR
	?RICE? OR ?WHEAT? OR ?PLANT?)
L37	6 SEA ABB=ON L34 AND ABC
L38	6 SEA ABB=ON L34 AND ABC 14 SEA ABB=ON L34 OR L36 OR L37 14 Cells from CA Pluce
	19 000
	•

Susan, I saved skri & L38, should you want any more done with it. M.J. => d ibib abs hitstr 138 1-14

L38 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:141200 HCAPLUS

DOCUMENT NUMBER: 142:254568

TITLE: Methods and compositions for increasing the efficacy

of biologically-active ingredients such as antitumor

agents

INVENTOR(S): Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.;

Thomas, Collin E.

PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA

SOURCE: PCT Int. Appl., 243 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

CN

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.					KIND DATE			APPLICATION NO.						DATE			
	WO	2005	0147	 77				2005	0217		WO 2	003 <i>-</i> 1	US32	667		2	0031	016
		W :	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
								DK,										
								IL,										
			LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,
	•		OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,
								UG,										
		RW:						MZ,									AZ,	BY,
			KG,	ΚZ,	MD,	RU,	TJ,	TM,	ΑT,	ΒE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
			FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
			BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
PRIO	RITY	APP	LN.	INFO	. :					,	US 2	002-	4188	03P		P 20	0021	016
AB	The	inv	enti-	on p	rovi	des r	neth	ods a	and (comp	ns.	for 1	modu.	lati	ng ti	he s	ensi	tivity
	of	cell	s to	cyt	otox:	ic c	pdmc	ls. a	nd o	ther	act	ive a	agen	ts.	In a	acco	rdan	ce with
	the	inv	enti-	on,	comp	ns. a	are	prov	ided	COM	pris	ing (comb.	inat.	ions	of		
								and a										
	age	nts	incl	ude (antil	oiot:	ics,	fung	gici	des,	her	bici	des,	ins	ecti	cide	s,	
	che	moth	erap	euti	c age	ents	, an	d pla	ant 9	grow	th r	egula	ator	s. I	Ву			
								acti						tion	allo	ows 1	use o	of
	COM	pns.	wit	h lo	were	d cor	ncns	. of	act	ive	ingr	edie	nts.					
ΙT				171														
	RL:	PAC	(Ph	arma	colo	gical	l ac	tivi	ty);	THU	(Th	erap	euti	c us	e);	BIOL		
	(Bi	_			_			ses)										
								inc				effi	cacy	of I	biol	act	tive	
		_					anti	tumo:	r ag	ents)							
RN	154	201-	55-5	HC	APLU:	5												

Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]-

4,5,6,7-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

RN171248-07-0 HCAPLUS

Benzeneacetic acid, 1-oxo-2-phenyl-1H-inden-3-yl ester (9CI) (CA INDEX CN

L38 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:722914 HCAPLUS

DOCUMENT NUMBER:

141:236625

TITLE:

Inhibitors of mycobacterial serine/threonine protein kinases for the treatment of mycobacterial infections

Pato, Janos; Keri, Gyorgy; Orfi, Laszlo; Waczek,

INVENTOR (S):

Frigyes; Horvath, Zoltan; Banhegyi, Peter; Szabadkai, Istavan; Marosfalvi, Jeno; Hegymegi-Barakonyi, Balint;

Szekelyhidi, Zsolt; Greff, Zoltan; Choidas, Axel;

Bacher, Gerald; Missio, Andrea; Koul, Anil

PATENT ASSIGNEE(S):

Hung.

SOURCE:

U.S. Pat. Appl. Publ., 51 pp., Cont.-in-part of Appl.

No. PCT/EP03/03697.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO	KIND DATE		APPLICATION NO.					DATE							
US 200417; WO 200209 WO 200209		A2 20		20040902 20021128 20031204			US 2003-715591 WO 2002-EP5573				20031118 20020521				
CC GI L: PI U	E, AG, O, CR, M, HR, S, LT, L, PT, A, UG,	CU, HU, LU, RO, US,	CZ, ID, LV, RU, UZ,	DE, IL, MA, SD, VN,	DK, IN, MD, SE, YU,	DM, IS, MG, SG, ZA,	DZ, JP, MK, SI, ZM,	EC, KE, MN, SK, ZW	EE, KG, MW, SL,	ES, KP, MX, TJ,	FI, KR, MZ, TM,	GB, KZ, NO, TN,	GD, LC, NZ, TR,	GE, LK, OM, TT,	GH, LR, PH, TZ,
K(G)	H, GM, G, KZ, R, IE, N, GQ,	MD, IT,	RU, LU,	TJ, MC,	TM,	AT, PT,	BE, SE,	CH, TR,	CY,	DE,	DK,	ES,	FI,	FR,	GB,
WO 2003084	1947		A1		2003	1016	7	WO 2	003-	EP36	97		20	0030	409
C	E, AG, D, CR, M, HR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
PI UZ RW: GI KO F:	5, LT, L, PT, A, UG, H, GM, G, KZ, I, FR, F, BJ,	RO, US, KE, MD, GB,	RU, UZ, LS, RU, GR,	SC, VC, MW, TJ, HU,	SD, VN, MZ, TM, IE,	SE, YU, SD, AT, IT,	SG, ZA, SL, BE, LU,	SK, ZM, SZ, BG, MC,	SL, ZW TZ, CH, NL,	TJ, UG, CY, PT,	TM, ZM, CZ, RO,	TN, ZW, DE, SE,	TR, AM, DK, SI,	TT, AZ, EE, SK,	TZ, BY, ES, TR,

EP 2001-112289 20010518 PRIORITY APPLN. INFO.: Α 20010522 US 2001-292325P Р Ρ 20010619 US 2001-298902P Α 20010627 EP 2001-115508 EP 2002-7923 A 20020409 WO 2002-EP5573 A2 20020521 WO 2003-EP3697 A2 20030409

OTHER SOURCE(S): MARPAT 141:236625

AB Mycobacterial serine/threonine protein kinases, particularly protein kinase G (PknG), are effective therapeutic targets for the treatment of mycobacterial infections. The invention discloses the use of mycobacterial serine/threonine protein kinases for developing methods for detection and determination of these kinases for recognizing and monitoring diseases and for controlling therapy of diseases. Addnl. disclosed are 4,5,6,7-tetrahydrobenzo[b]thiophene compds., benzo[g]quinoxaline compds., and pharmaceutically acceptable salts thereof, and methods of using such compds. and salts thereof for the prophylaxis and/or treatment of virally and/or bacterially induced infections, particularly mycobacteria-induced infections, including opportunistic infections, as well as pharmaceutical compns. containing at least one 4,5,6,7-tetrahydrobenzo[b]thiophene compound and/or benzo[g]quinoxaline compound and/or pharmaceutically acceptable salts thereof in a pharmaceutically acceptable carrier.

IT 296266-55-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(inhibitors of mycobacterial serine/threonine protein kinases for treatment of mycobacterial infections)

RN 296266-55-2 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]-4,5,6,7-tetrahydro-7-oxo-, ethyl ester (9CI) (CA INDEX NAME)

L38 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:818414 HCAPLUS

DOCUMENT NUMBER: 139:317414

TITLE: 4,5,6,7-tetrahydrobenzo[b] thiophene derivatives and

methods for medical intervention against mycobacterial

infections

INVENTOR(S): Missio, Andrea; Bacher, Gerald; Koul, Anil; Choidas,

Axel

PATENT ASSIGNEE(S): Axxima Pharmaceuticals A.-G., Germany

SOURCE: PCT Int. Appl., 94 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

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PATENT NO.
                       KIND
                              DATE
                                         APPLICATION NO.
                                                                DATE
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                                       WO 2003-EP3697
    WO 2003084947
                              20031016
                                                                20030409
                        A1
           AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    EP 1492783
                        A1
                             20050105 EP 2003-720441
                                                               20030409
           AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
    US 2004171603
                                                                20031118
                        A1
                              20040902
                                         US 2003-715591
                                          EP 2002-7923
PRIORITY APPLN. INFO.:
                                                             A 20020409
                                          EP 2001-112289
                                                            A 20010518
                                          US 2001-292325P
                                                            P 20010522
                                          US 2001-298902P
                                                            P 20010619
                                          EP 2001-115508
                                                            A 20010627
                                          WO 2002-EP5573
                                                            A2 20020521
                                          WO 2003-EP3697
                                                             W 20030409
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OTHER SOURCE(S): MARPAT 139:317414

The invention describes 4,5,6,7-tetrahydrobenzo[b] thiophene derivs. and pharmaceutically acceptable salts thereof, the use of these derivs. for the prophylaxis and/or treatment of mycobacteria-induced infections and opportunistic infections, as well as compns. containing at least one 4,5,6,7-tetrahydrobenzo[b] thiophene derivative and/or pharmaceutically acceptable salt thereof. Compds. of the invention are used as inhibitors of protein kinases, e.g. Mycobacterium tuberculosis protein kinase G. The invention also discloses the use of a protein serine/threonine kinase for developing methods for detection and determination of such a kinase for recognizing and monitoring diseases and for controlling therapy of diseases.

IT 296266-55-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(tetrahydrobenzothiophene derivs. for treatment of mycobacterial and opportunistic infections, and diagnostic and screening methods)

RN 296266-55-2 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]-4,5,6,7-tetrahydro-7-oxo-, ethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L38 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
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ACCESSION NUMBER: 2003:23438 HCAPLUS

DOCUMENT NUMBER: 138:68713

TITLE: Modulating resistance of tumor and pathogen cells to

foreign compounds by manipulation of ATP gradients via

regulation of ABC transporters and

ecto-phosphatases

INVENTOR(S): Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.

PATENT ASSIGNEE(S): University of Texas, USA

SOURCE: U.S. Pat. Appl. Publ., 41 pp., Cont.-in-part of U.S.

Ser. No. 261,825. CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PAT	ENT	NO.			KIN	D	DATE		i	APPL	I CAT	ION 1	. 01		D	ATE	
						-									-		
US	2003	0083	59		A1		2003	0109	1	US 2	002-	1340	19		2	0020	425
US	2002	0069	01		A1		2002	0117	1	US 1	999-2	2447	92		1:	9990:	205
WO	2003	0914	03		A2		2003	1106	1	WO 2	003-1	JS12'	780		2	0030	425
WO	2003	0914	03		A3		2004	1104									
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	ĎΖ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
		PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,
		TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW					
	RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
		KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
PRIORITY	APP	LN.	INFO	. :					1	US 1	999-2	2447	92	1	A2 1	9990:	205
									1	US 1	999-2	26182	25		A2 1	9990	303
									1	US 2	002-	1340	19	1	A1 2	0020	425

The present invention relates to methods for modulating the growth of ΔR tumor and pathogen cells and the resistance of cells to foreign compds., i.e. drugs, antibiotics, etc. by altering the ATP gradient across biol. membranes. The altering of the ATP gradient across biol. membranes is achieved through the manipulation of ecto-phosphatase (e.g., human apyrase) activity and ABC transporter mol. (e.g., Arabidopsis AtPGP-1) activity which may also be useful to confer herbicide resistance to plants, confer antibiotic resistance to bacteria, confer drug resistance to yeast cells, or to reduce resistance in cells to facilitate chemotherapeutic treatments, and to reduce resistance in bacteria and yeast. The present invention is also directed to the methods for identifying ecto-phosphatase inhibitors and uses thereof. Nineteen ecto-phosphatase inhibitory mols. are provided which are useful in reversing multi-drug resistance in Arabidopsis and yeast.

IT 154201-55-5 171248-07-0

RL: AGR (Agricultural use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC

transporters and ecto-phosphatases)

RN 154201-55-5 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]-

4,5,6,7-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

171248-07-0 HCAPLUS RN

Benzeneacetic acid, 1-oxo-2-phenyl-1H-inden-3-yl ester (9CI) (CA INDEX CN

L38 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

2002:833490 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 137:306061

TITLE: Pesticidal and herbicidal activity through modulation

of animal and plant cell membrane transport

INVENTOR (S):

Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.

PATENT ASSIGNEE(S): Board of Regents, The University of Texas System, USA

SOURCE: U.S. Pat. Appl. Publ., 41 pp., Cont.-in-part of U.S.

Ser. No. 244,791.

CODEN: USXXCO

Patent DOCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	APPLICATION NO.				
				· -				
US 2002160915	A1	20021031	US 2001-793336		20010226			
US 6448472	B1	20020910	US 1999-244791		19990205			
PRIORITY APPLN. INFO.:			US 1999-244791	A2	19990205			
			US 2000-185299P	P	20000228			

The present invention relates to the modulation of pesticidal and AB herbicidal activity by treatment of a membrane transport system in a cell. This entails modifying the extra-cellular phosphatases found in the membranes of these cells. By modifying the ATP gradient across the biol. membrane of a target plant, bacteria, insect or mammalian cell via inhibiting one or more extra-cellular phosphatases, it is possible to alter the sensitivity to a pesticide or herbicide. The method also comprises inhibiting an ABC transporter in the target cell. The method can also be used for identifying chems. with pesticidal activity.

ΙT 154201-55-5 171248-07-0

RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL

(Biological study); USES (Uses)

(ectophosphatase inhibitor which enhances

pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes)

RN 154201-55-5 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]-4,5,6,7-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

RN 171248-07-0 HCAPLUS

CN Benzeneacetic acid, 1-oxo-2-phenyl-1H-inden-3-yl ester (9CI) (CA INDEX NAME)

L38 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:185280 HCAPLUS

DOCUMENT NUMBER: 136:244034

TITLE: Method for increasing the effectiveness of

antiinfective agents by inhibiting ecto-phosphatase

and/or ABC transporter activities

INVENTOR(S): Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.

PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA

SOURCE: PCT Int. Appl., 65 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Facent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT		KIND DA		DATE APPLICATION NO.						DATE						
WO 2002020726				A2 20020314			1	WO 2001-US28242						20010907		
WO 2002020726				A3		20020606										
W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PH,	PL,
	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	ΤZ,	UA,	ŪĠ,
	US,	UZ,	VN,	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM	
RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG 20020322 AU 2001090710 **A5** AU 2001-90710 20010907 US 2002077365 A1 20020620 US 2001-949268 20010907 US 2000-231088P 20000908 PRIORITY APPLN. INFO.: W 20010907 WO 2001-US28242

GT

Ι

AB The present invention relates to methods for decreasing the resistance of microbial strains to antiinfectives such an antibiotics and antifungals by altering the ATP gradient across biol. membranes. The altering of the ATP gradient across biol. membranes is achieved through the inhibition of ecto-phosphatase activity and/or ABC transporter mol. activity which may be useful to reduce resistance in bacteria and yeast to aid in the treatment of certain infections and disease and to lower the concentration of

antiinfectives necessary to inhibit the growth of microbial strains. Apyrase inhibitor I increased the growth inhibitory effect of the fungicide chlorothalonil by over 50%. Surflan was an equally effective weed killer against Arabidopsis thaliana at a five-fold less concentration in

presence of II.

the

IT 154201-55-5 171248-07-0

RL: BSU (Biological study, unclassified); CST (Combinatorial study, unclassified); BIOL (Biological study); CMBI (Combinatorial study) (as apyrase inhibitor; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities)

RN 154201-55-5 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]-4,5,6,7-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

RN 171248-07-0 HCAPLUS

CN Benzeneacetic acid, 1-oxo-2-phenyl-1H-inden-3-yl ester (9CI) (CA INDEX NAME)

L38 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:676991 HCAPLUS

DOCUMENT NUMBER: 135:222868

TITLE: Pesticide adjuvant activity through modulation of

animal and plant cell membrane transport

INVENTOR(S): Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.

PATENT ASSIGNEE(S): Board of Regents of the University of Texas System,

USA

SOURCE: PCT Int. Appl., 76 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 2001066792	A1 20010913	WO 2001-US7423	20010307
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BY, 1	BZ, CA, CH, CN,
CR, CU, CZ,	DE, DK, DM, DZ,	EE, ES, FI, GB, GD, G	GE, GH, GM, HR,
HU, ID, IL,	IN, IS, JP, KE,	KG, KP, KR, KZ, LC,	LK, LR, LS, LT,
LU, LV, MA,	MD, MG, MK, MN,	MW, MX, MZ, NO, NZ,	PL, PT, RO, RU,
SD, SE, SG,	SI, SK, SL, TJ,	TM, TR, TT, TZ, UA, I	UG, UZ, VN, YU,
ZA, ZW, AM,	AZ, BY, KG, KZ,	MD, RU, TJ, TM	
RW: GH, GM, KE,	LS, MW, MZ, SD,	SL, SZ, TZ, UG, ZW, Z	AT, BE, CH, CY,
DE, DK, ES,	FI, FR, GB, GR,	IE, IT, LU, MC, NL,	PT, SE, TR, BF,
BJ, CF, CG,	CI, CM, GA, GN,	GW, ML, MR, NE, SN,	TD, TG
US 2002103082	A1 20020801	US 2001-800327	20010306
CA 2373424	AA 20010913	CA 2001-2373424	20010307
PRIORITY APPLN. INFO.:		US 2000-187819P	P 20000308
		US 2001-800327	A 20010306
		WO 2001-US7423	W 20010307

AB The invention relates to the modulation of pesticidal and herbicidal activity by treatment of a membrane transport system in a cell. This entails modifying the extracellular phosphatases found in the membranes of

these cells. By modifying the ATP gradient across the biol. membrane of a target **plant**, bacteria, insect or mammalian cell via inhibiting one or more extracellular phosphatases, it is possible to alter the sensitivity to a pesticide or herbicide. In preferred embodiments, the chemical moieties of the invention act as adjuvants to enhance pesticidal activity.

IT 154201-55-5 171248-07-0

RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses) (pesticide adjuvant acting by inhibition of extracellular phosphatases in membranes)

RN 154201-55-5 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]4,5,6,7-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

RN 171248-07-0 HCAPLUS

CN Benzeneacetic acid, 1-oxo-2-phenyl-1H-inden-3-yl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2001:661570 HCAPLUS

DOCUMENT NUMBER:

135:206922

TITLE:

Pesticidal and herbicidal activity through modulation

of animal and plant cell membrane transport

INVENTOR (S):

Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.

PATENT ASSIGNEE(S):

Board of Regents, the University of Texas System, USA

SOURCE: PCT Int. Appl., 74 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:
FAMILY ACC. NUM. COUNT:

English

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2001064859 A1 20010907 WO 2001-US6503 20010227

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,

BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.: US 2000-185299P P 20000228

AB The invention relates to the modulation of pesticidal and herbicidal activity by treatment of a membrane transport system in a cell. This entails modifying the extra-cellular phosphatases found in the membranes of these cells. By modifying the ATP gradient across the biol. membrane of a target plant, bacteria, insect or mammalian cell via inhibiting one or more extracellular phosphatases, it is possible to alter the sensitivity to a pesticide or herbicide. The method also comprises inhibiting an ABC transporter in the target cell. The method can also be used for identifying chems. with pesticidal activity.

IT 154201-55-5 171248-07-0

RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(ectophosphatase inhibitor which enhances

pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes)

RN 154201-55-5 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]4,5,6,7-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

RN 171248-07-0 HCAPLUS

CN Benzeneacetic acid, 1-oxo-2-phenyl-1H-inden-3-yl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2000:628251 HCAPLUS

DOCUMENT NUMBER:

133:219782

TITLE:

Genetic and epigenetic manipulation of ABC

transporters and ecto-phosphatases for modulating drug

resistance and methods for detection of ecto-

phosphatase inhibitors

INVENTOR(S):
Thomas, Collin E.; Windsor, J. Brian; Roux, Stan J.;

Lloyd, Alan M.; Hurley, Laurence

PATENT ASSIGNEE(S): University of Texas, USA SOURCE: PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO	•	K	IND	DATE	APPLICATION NO.	DATE				
WO 200005	2144	_	Å1 20000908		WO 2000-US5315	20000228				
W: A	E, AL,	AM, A	T, AU,	, AZ, BA,	BB, BG, BR, BY, CA,	CH, CN, CR, CU,				
C	Z, DE,	DK, D	M, EE,	, ES, FI,	GB, GD, GE, GH, GM,	HR, HU, ID, IL,				
I	N, IS,	JP, K	E, KG,	, KP, KR,	KZ, LC, LK, LR, LS,	LT, LU, LV, MA,				
M	D, MG,	MK, M	IN, MW,	, MX, NO,	NZ, PL, PT, RO, RU,	SD, SE, SG, SI,				
S	K, SL,	TJ, T	M, TR,	, TT, TZ,	UA, UG, UZ, VN, YU,	ZW, AM, AZ, BY,				
K	G, KZ,	MD, R	U, TJ,	, TM						
RW: G	H, GM,	KE, L	S, MW,	, SD, SL,	SZ, TZ, UG, ZW, AT,	BE, CH, CY, DE,				
D	K, ES,	FI, F	R, GB,	, GR, IE,	IT, LU, MC, NL, PT,	SE, BF, BJ, CF,				
C	G, CI,	CM, G	A, GN,	, GW, ML,	MR, NE, SN, TD, TG					
EP 118562	3		A1	20020313	EP 2000-913685	20000228				
R: A	T, BE,	CH, D	E, DK,	, ES, FR,	GB, GR, IT, LI, LU,	NL, SE, MC, PT,				
I	E, SI,	LT, L	V, FI,	, RO						
US 200217	3031		A1	20021121	US 2002-47251	20020114				
PRIORITY APPLN	. INFO.	. :			US 1999-261825	A 19990303				
					WO 2000-US5315	W 20000228				

AB The present invention relates to methods for modulating the resistance of cells to foreign compds., i.e. drugs, antibiotics, etc. by altering the ATP gradient across biol. membranes. Altering the ATP gradient across biol. membranes is achieved through the manipulation of ecto-phosphatase activity and ABC transporter mol. activity. The above method may be useful to confer herbicide resistance to plants, antibiotic resistance to bacteria, and drug resistance to yeast cells, or to reduce resistance in cells, bacteria, and yeast in order to facilitate chemotherapeutic treatments. The present invention is also directed to the methods for identifying ecto-phosphatase inhibitors and uses thereof. Thus, Arabidopsis thaliana has been shown to possess an ecto-apyrase and this ecto-apyrase and PGP-1 (an MDR-like protein) to have a role in MDR. Addnl., the extracellular ATP pool was shown to be critical for MDR in yeast. Screening of a combinatorial library of small mols. has resulted in identification of apyrase inhibitors.

IT 154201-55-5 171248-07-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(genetic and epigenetic manipulation of ABC transporters and ecto-phosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors)

RN 154201-55-5 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]-4,5,6,7-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

171248-07-0 HCAPLUS RN

Benzeneacetic acid, 1-oxo-2-phenyl-1H-inden-3-yl ester (9CI) (CA INDEX CN NAME)

REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:838034 HCAPLUS

DOCUMENT NUMBER: 124:8370

TITLE: Synthesis of O-acyl derivatives of

2-aryl-1H-indene-1,3(2H)-diones and

2-aryl-2,3-dihydrophenalene-1,3-diones

AUTHOR (S): Stoyanov, N.; Nedev, H.; Minchev, S.

CORPORATE SOURCE: Department of Chemistry, Biotechnology Institute,

Razgrad, 7200, Bulg.

SOURCE: Dokladi na Bulgarskata Akademiya na Naukite (1994),

47(9), 41-3

CODEN: DBANEH; ISSN: 0861-1459

PUBLISHER: Izdatelstvo na Bulgarskata Akademiya na Naukite

DOCUMENT TYPE: Journal LANGUAGE: English

AB The preparation of the title compds. are discussed.

IT 171248-07-0P 171248-10-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of 0-acyl derivs. of 2-aryl-1H-indene-1,3(2H)-diones and 2-aryl-2,3-dihydrophenalene-1,3-diones)

RN 171248-07-0 HCAPLUS

CN Benzeneacetic acid, 1-oxo-2-phenyl-1H-inden-3-yl ester (9CI) (CA INDEX NAME)

RN 171248-10-5 HCAPLUS

L38 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1994:244500 HCAPLUS

DOCUMENT NUMBER:

120:244500

TITLE:

Synthesis and local anesthetic activity of some 2-aminoacetylamino-3-carbethoxy/anilido-4,5,6,7-

tetrahydrobenzo[b]thiophenes

AUTHOR (S):

Gadad, A. K.; Kumar, Hemant; Shishoo, C. J.; Khazi, I.

M.; Mahajanshetti, C. S.

CORPORATE SOURCE:

Dep. Pharm. Chem., Coll. Pharm., Belgaum, 590 010,

India

SOURCE:

Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1994),

33B(3), 298-301

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

AB Twenty new 2-substituted aminoacetylamino-3-carbethoxy/anilido-4,5,6,7-tetrahydrobezo[b]thiophenes (I, R = CO2Et, CONHPh, CONHC6H4Me-o; R1 = Me2N, Et2N, piperidino, morpholino, piperazino, 1-pyrrolidinyl, cyclohexylamino) were synthesized with a view to studying the effect of structural modification of carticaine on the local anesthetic activity and were evaluated by Sollman's method as well as Bulbring and Wajda method using lignocaine hydrochloride as a standard All the tested compds. show moderate to good activity.

IT 154201-55-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and local anesthetic activity of)

RN 154201-55-5 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]-4,5,6,7-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

L38 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:448485 HCAPLUS

DOCUMENT NUMBER: 117:48485

TITLE: Novel synthesis of thieno[2,3-d]pyrimidines AUTHOR(S): Shaban, M. A.; Mohamed, M. S.; Kamel, M. M.;

El-Zanfally, S. H.

CORPORATE SOURCE: Fac. Pharm., Cairo Univ., Cairo, Egypt

SOURCE: Bulletin of the Faculty of Pharmacy (Cairo University)

(1990), 28(1), 17-19

CODEN: BFPHA8; ISSN: 0575-1373

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:48485

GI

AB The reaction of 2-amino-4,5,6,7-tetrahydrobenzo[b]thiophene-3-carboxamide
(I) with 1,2-dielectrophilic reagents has been investigated. Fusion of I
and benzoin gave the thienopyrimidine derivative II (R = Ph). A mechanism for
its formation was postulated, and confirmed by reacting I with
benzaldehyde. The least reaction is the basis of a novel synthesis for
thienopyrimidines.

IT 142354-81-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 142354-81-2 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 4,5,6,7-tetrahydro-2-[[(phenylamino)acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

L38 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1

1979:121287 HCAPLUS

DOCUMENT NUMBER:

90:121287

TITLE:

Esters of 3-hydroxyindone compounds as herbicides and

miticides

INVENTOR (S):

Durden, John A., Jr.; Sousa, Anthony A.; Stephen, John

F

PATENT ASSIGNEE(S):

Union Carbide Corp., USA

SOURCE:

U.S., 18 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
				•	
US 4104043 🗸	Α	19780801	US 1972-314370		19721212
IN 138958	Α	19760417	IN 1973-CA392		19730221
CA 1030976	A1	19780509	CA 1973-185629		19731113
DE 2361084	A1	19740620	DE 1973-2361084		19731207
DE 2361084	C2	19841025			
AU 7363395	A1	19750612	AU 1973-63395		19731210
BE 808486	A1	19740611	BE 1973-138738		19731211
FR 2209742	A1	19740705	FR 1973-44143		19731211
JP 49094828	A2	19740909	JP 1973-137454		19731211
JP 59020642	B4	19840515			
BR 7309691	A0	19741022	BR 1973-9691		19731211
ZA 7309408	A	19741030	ZA 1973-9408		19731211
GB 1403477	Α	19750820	GB 1973-57322		19731211
ES 421344	A1	19760416	ES 1973-421344		19731211
CH 590611	A	19770815	CH 1973-17328		19731211
IL 43801	A1	19780615	IL 1973-43801		19731211
US 4091006	Α	19780523	US 1975-618837		19751001
PRIORITY APPLN. INFO.:			US 1972-314370	Α	19721212
GI					

$$R^{5}$$

Ι

One hundred thirty title esters I (R = H, halo or an organic moiety; H, halo, Me, Et, MeO, EtO, CCl3, CF3, CCl2F, CClF2; Rl = H, halo, alkyl, alkoxy, NO2, CCl3, CF3, amido; R3 = halo, Me, Et, MeO, EtO; R4 = H, alkyl, haloalkyl, alkoxy, amido, halo; R5 = H, halo, alkyl, alkoxy, CF3, CCl3, CCl2F, CClF2, amido; n = 1-4; R1R4, R2R4 = CH:CHCH:CH) were prepared and each was evaluated for its herbicidal and/or miticidal activity. Tabulation of compds. with only 1 variable permitted evaluation of the effect of the structure on the biol. activity. Thus, treatment of 2-(2,6-dichlorophenyl)-1,3-indandione with BzCl in pyridine gave 33% I (R = Ph, R1 = R3 = Cl, R2 = R4 = R5 = H), which gave 100% kill of adult mites and mite ova in standard tests and had a herbicide rating of 31/40.

IT 53083-25-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and acaricidal and herbicidal activity of)

RN 53083-25-3 HCAPLUS

CN Benzeneacetic acid, 1-oxo-2-(2,4,6-trimethylphenyl)-1H-inden-3-yl ester (9CI) (CA INDEX NAME)

L38 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1974:477734 HCAPLUS

DOCUMENT NUMBER: 81:77734

TITLE: Substituted 3-hydroxyindones

INVENTOR(S): Durden, John A., Jr., Sousa, Anthony A., Stephen, John

F.

PATENT ASSIGNEE(S): Union Carbide Corp. SOURCE: Ger. Offen., 87 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2361084	A1	19740620	DE 1973-2361084		19731207
DE 2361084	C2	19841025			
US 4104043	Α	19780801	US 1972-314370		19721212
PRIORITY APPLN. INFO.:			US 1972-314370	A	19721212
GI For diagram(s), see	printe	d CA Issue.			
AB 2-Phenyl-3-hydroxyi	ndenone	esters I (R	= e.g., Me, Ph, Me2N	Η,	Me3C; R1,
R2, and $R3 = e.g.$,	H, Me,	Cl, NO2, MeO), useful as acaricid	es	and
pre-emergent herbic	ides, w	ere prepared	by the reaction of a		

2-phenyl-1,3-indandione with an acid chloride or anhydride. Thus, 2-(2,4,6-trimethylphenyl)-1,3-indandione reacted with Ac2O to give I (R=R1=R2=R3=Me). About 115 I were prepared

IT 53083-25-3 53083-48-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(acaricidal and herbicidal activity of)

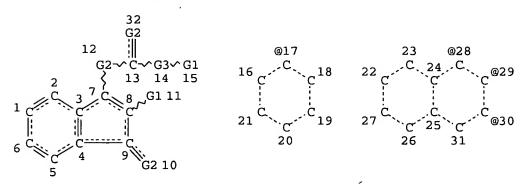
RN 53083-25-3 HCAPLUS

CN Benzeneacetic acid, 1-oxo-2-(2,4,6-trimethylphenyl)-1H-inden-3-yl ester (9CI) (CA INDEX NAME)

RN 53083-48-0 HCAPLUS

CN Benzeneacetic acid, 2,4-dichloro-, 1-oxo-2-(2,4,6-trimethylphenyl)-1H-inden-3-yl ester (9CI) (CA INDEX NAME)

=> d que stat 138 L18 STR



VAR G1=17/28/29/30

VAR G2=O/S

REP G3 = (1-5) CH2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

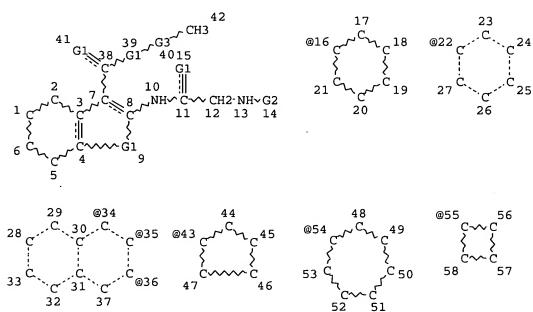
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE

L20 4 SEA FILE=REGISTRY SSS FUL L18 L21 10 SEA FILE=HCAPLUS ABB=ON L20

L30 STR



VAR G1=O/S

VAR G2=16/22/34/35/36/43/54/55

REP G3 = (1-4) CH2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 58

STEREO ATTRIBUTES: NONE									
L32 1	28 SEA FILE=REGISTRY SSS FUL L30								
L33	11 SEA FILE=HCAPLUS ABB=ON L32								
L34	14 SEA FILE=HCAPLUS ABB=ON L21 OR L33								
L35	1 SEA FILE=REGISTRY ABB=ON PHOSPHATASE/CN								
L36	7 SEA FILE=HCAPLUS ABB=ON L34 AND ((L35 OR ?PHOSPHATAS?)(W)?INHI								
	BIT? OR (?DRUG?(W)?RESIST?)(4A)(?DECREAS? OR ?INHIBIT? OR								
	?LESSEN? OR ?PREVENT? OR ?CONTROL?) OR ?PEAS? OR ?CARROT? OR								
	?FLOWER? OR ?RICE? OR ?WHEAT? OR ?PLANT?)								
L37	6 SEA FILE=HCAPLUS ABB=ON L34 AND ABC								
L38	14 SEA FILE=HCAPLUS ABB=ON L34 OR L36 OR L37								

Hanley 10/047,251

26/04/2005

=> d ibib abs hitstr l12 1-1

L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2000:628251 HCAPLUS

DOCUMENT NUMBER:

133:219782

TITLE:

Genetic and epigenetic manipulation of ABC

transporters and ecto-phosphatases for modulating drug

resistance and methods for detection of

ecto-phosphatase inhibitors

INVENTOR(S):

Thomas, Collin E.; Windsor, J. Brian

; Roux, Stan J.; Lloyd, Alan M.;

Hurley, Laurence

PATENT ASSIGNEE(S):

University of Texas, USA PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

SOURCE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.					KIND		DATE		APPLICATION NO.						DATE			
	WO	WO 2000052144				A1		20000908		WO 2000-US5315					20000228				
		W:	ΑE,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,	
			CZ,	DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	
			IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	
			MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	
			SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	UZ,	VN,	YU,	ZW,	AM,	ΑZ,	BY,	
			KG,	KZ,	MD,	RU,	TJ,	TM											
		RW:	GH,	GM,	ΚE,	LS,	MW,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	DE,	
			DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	
			CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG					
	EP 1185623					A1		2002	0313	EP 2000-913685					20000228				
		R:	ΑT,	ΒE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FI,	RO											
US 2002173031					A1		20021121 US 2002-47251							2	0020	114			
PRIORITY APPLN. INFO.:								US 1999-261825				1	A 1	9990	303				
										1	WO 2	000-1	US53	15	1	W 2	0000	228	
							_				_				_				

- AB The present invention relates to methods for modulating the resistance of cells to foreign compds., i.e. drugs, antibiotics, etc. by altering the ATP gradient across biol. membranes. Altering the ATP gradient across biol. membranes is achieved through the manipulation of ecto-phosphatase activity and ABC transporter mol. activity. The above method may be useful to confer herbicide resistance to plants, antibiotic resistance to bacteria, and drug resistance to yeast cells, or to reduce resistance in cells, bacteria, and yeast in order to facilitate chemotherapeutic treatments. The present invention is also directed to the methods for identifying ecto-phosphatase inhibitors and uses thereof. Thus, Arabidopsis thaliana has been shown to possess an ecto-apyrase and this ecto-apyrase and PGP-1 (an MDR-like protein) to have a role in MDR. Addnl., the extracellular ATP pool was shown to be critical for MDR in yeast. Screening of a combinatorial library of small mols. has resulted in identification of apyrase inhibitors.
- IT 50-81-7, Ascorbic acid, uses 11098-84-3, Ammonium
 molybdate
 - RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (genetic and epigenetic manipulation of ABC transporters and ecto-phosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors)

RN 50-81-7 HCAPLUS

CN L-Ascorbic acid (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 11098-84-3 HCAPLUS

CN Ammonium molybdenum oxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 9013-05-2, Phosphatase 41481-51-0 139963-64-7

154201-55-5 168832-50-6 171248-07-0

291536-79-3 291536-80-6 291536-81-7

291536-82-8 291536-83-9 291536-84-0

291536-85-1 291536-86-2 291536-87-3

291536-88-4 291536-89-5 291536-90-8

291536-91-9 291536-92-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)

(genetic and epigenetic manipulation of ABC transporters and

ecto-phosphatases for modulating drug resistance and methods for

detection of ecto-phosphatase inhibitors)

RN 9013-05-2 HCAPLUS

CN Phosphatase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 41481-51-0 HCAPLUS

CN Guanidine, N,N-dibutyl-N'-phenyl-N''-[(phenylamino)sulfonyl]- (9CI) (CA INDEX NAME)

RN 139963-64-7 HCAPLUS

CN Ethanone, 2,2'-thiobis[1-(1H-indol-3-yl)- (9CI) (CA INDEX NAME)

RN 154201-55-5 HCAPLUS

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]-4,5,6,7-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

RN 168832-50-6 HCAPLUS

CN Octanediamide, N,N'-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 171248-07-0 HCAPLUS

CN Benzeneacetic acid, 1-oxo-2-phenyl-1H-inden-3-yl ester (9CI) (CA INDEX NAME)

RN 291536-79-3 HCAPLUS

CN Benzenamine, N-(3-hexyl-4-phenyl-2(3H)-thiazolylidene)-, monohydrobromide (9CI) (CA INDEX NAME)

HBr

291536-80-6 HCAPLUS RN

CN [1,1'-Biphenyl]-4-sulfonamide, N-(3-methylphenyl)- (9CI) (CA INDEX NAME)

RN 291536-81-7 HCAPLUS

CN Benzamide, 4-chloro-N-(3-chlorophenyl)-N-[(2,4-dichlorophenyl)methyl]-(9CI) (CA INDEX NAME)

RN 291536-82-8 HCAPLUS

CN 1-Naphthaleneacetic acid, [(2-hydroxy-5-methylphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

291536-83-9 HCAPLUS RN

Benzamide, N-(4a,8a-dihydro-1-naphthalenyl)-3,5-bis(1,1-dimethylethyl)-CN(9CI) (CA INDEX NAME)

RN291536-84-0 HCAPLUS

CN 1-Naphthaleneacetic acid, [(4-bromophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 291536-85-1 HCAPLUS

CN Benzoic acid, 3-methyl-, [1-(2-naphthalenyl)ethylidene]hydrazide (9CI) (CA INDEX NAME)

RN 291536-86-2 HCAPLUS

CN Benzoic acid, 2-[[(4-chlorophenyl)amino]carbonyl]-, 2-propynyl ester (9CI) (CA INDEX NAME)

RN 291536-87-3 HCAPLUS

CN Acetic acid, (2,4,6-trimethylphenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

$$\begin{picture}(20,10) \put(0,0){\line(1,0){100}} \put(0,0){\line(1,0){10$$

291536-88-4 HCAPLUS RN

2H-1-Benzopyran-3-carbothioic acid, 2-oxo-, S-heptyl ester (9CI) (CA CNINDEX NAME)

RN 291536-89-5 HCAPLUS

CNHexanoic acid, [(2-hydroxy-5-nitrophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

$$CH = N-NH-C-(CH2)4-Me$$

$$NO2$$

291536-90-8 HCAPLUS RN

4-Thiazolidinone, 3-[[(4-methoxyphenyl)amino]methyl]-2-methylene-5-[(4-CN nitrophenyl) methylene] - (9CI) (CA INDEX NAME)

RN 291536-91-9 HCAPLUS

CN Benzamide, 3-[[(4-bromophenyl)amino]sulfonyl]-N-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 291536-92-0 HCAPLUS

CN Acetic acid, phenoxy-, 1-[(benzoylamino)methyl]-2-naphthalenyl ester (9CI) (CA INDEX NAME)

IT 56-65-5, ATP, biological studies

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(gradient of; genetic and epigenetic manipulation of ABC transporters and ecto-phosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors)

RN 56-65-5 HCAPLUS

Adenosine 5'-(tetrahydrogen triphosphate) (8CI, 9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

REFERENCE COUNT:

8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



STIC Search Report Biotech-Chem Library

STIC Database Tracking Number: 151080

TO: Susan Hanley Location: 3d70 / 3e71 Tuesday, April 26, 2005

Art Unit: 1651

Phone: 571-272-2508

Serial Number: 10 / 047251

From: Jan Delaval

Location: Biotech-Chem Library

Remsen 1a51

Phone: 571-272-22504

jan.delaval@uspto.gov

Search Notes		
	·	
		-



W/047, 25/

Search Rennest:

- 1. Please do a structure search for each of the attached compounds with the modifications that I have specified. Where possible, I have indicated a structural feature common to all of the attached compounds so that you may be able to consolidate the compounds into the fewest searches possible.
- 2. Please see if the compounds from your search results have been used in the following methods:
- a. Does the compound inhibit any phosphatase?
- b. Does the compound decrease drug resistance in plants or mammals?
- c. Have the compounds ever been administered (i.e. sprayed, applied, etc.) to a plant such as peas, carrots, flowers, rice, wheat, any plant that you can think of.
- d. Have any of the compounds been used to inhibit (down-regulate, antagonist, etc) an ABC transporter (also known as an ABC-binding cassette) in a cell?

For the plants, the plant can be in a cell culture.

Thanks. Please call me if you have any questions 2-2508.

Susan

open for substitution

(138

VI

Open for substitution

(149)

HO

HO

HO

HO

HSH/8H

napthylor NH Off any substitutions on ring

25451225.1 10 LUI

X or open to substitution

X or only answb. alkyl group

N-NH

any unsubstituted ackyl

any unsubstituted ackyl

any unsubstituted ackyl

any or tho, we to or para

peace open or o o o o halogen sub. or tho, meta o or H pana

=> fil reg FILE 'REGISTRY' ENTERED AT 08:49:31 ON 26 APR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 APR 2005 HIGHEST RN 849177-50-0 DICTIONARY FILE UPDATES: 25 APR 2005 HIGHEST RN 849177-50-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

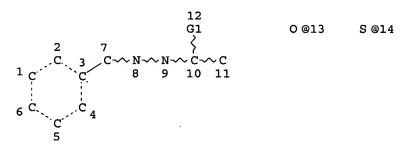
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que 138 L21 STR



VAR G1=13/14 NODE ATTRIBUTES: NSPEC IS RC AT 11 CONNECT IS E2 RC AT 8 CONNECT IS E2 RC AT 9 CONNECT IS E1 RC AT 13 CONNECT IS E1 RC AT 14 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 14

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STEREO ATTRIBUTES: NONE
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L23 241180 SEA FILE=REGISTRY SSS FUL L21

L24 STR

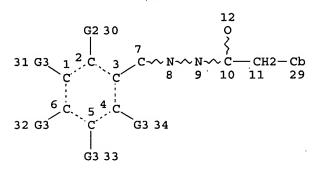
VAR G2=H/S/O
VAR G3=H/AK
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 29
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE L26 STR



VAR G2=H/S/O
VAR G3=H/AK
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 29
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 18

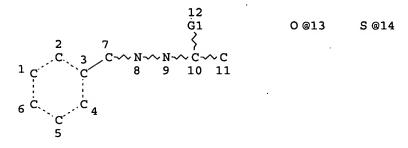
STEREO ATTRIBUTES: NONE

SIEREO AIIRIDOIES. NOME								
L28	229	SEA	FILE=REGISTRY	SUB=L23	CSS FUL	L24		
L29	130	SEA	FILE=REGISTRY	SUB=L28	SSS FUL	L26		
L30	26	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L29	AND	C6-C6/ES
L31	24	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L30	NOT	2 NAPHTHALENE?
L32	· 104	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L29	NOT	L30
L33	10	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L32	AND	NR>=3
L34	6	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L33	TOM	(C24H26N4O2 OR
		C191	H24N2O2 OR C25I	H28N2O4)				
L35	94	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L32	NOT	L33

Compound VI

L36 5 SEA FILE=REGISTRY ABB=ON PLU=ON L35 AND (C19H24N2O3 OR C15H16N2O OR C15H17N3O OR C20H26N2O3 OR C18H22N2O3)
L37 89 SEA FILE=REGISTRY ABB=ON PLU=ON L35 NOT L36
L38 119 SEA FILE=REGISTRY ABB=ON PLU=ON (L31 OR L34 OR L37)

=> d sta que 145 L21 STR



VAR G1=13/14

NODE ATTRIBUTES:

NSPEC IS RC AT 11

CONNECT IS E2 RC AT 8

CONNECT IS E2 RC AT 9

CONNECT IS E1 RC AT 13

CONNECT IS E1 RC AT 14

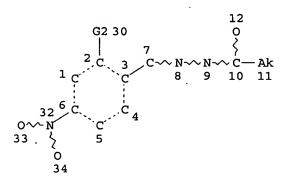
DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L23 241180 SEA FILE=REGISTRY SSS FUL L21 L39 STR



VAR G2=H/S/O NODE ATTRIBUTES: CONNECT IS M1 RC AT 33 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 3
NUMBER OF NODES IS

STEREO ATTRIBUTES: NONE L42 STR

VAR G2=H/S/O NODE ATTRIBUTES: CONNECT IS E1 RC AT 11 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 3

NUMBER OF NODES IS 16

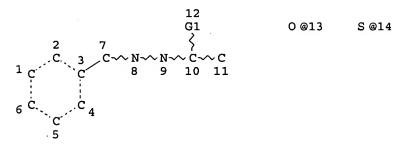
STEREO ATTRIBUTES: NONE

L44 75 SEA FILE=REGISTRY SUB=L23 SSS FUL L42 L45 17 SEA FILE=REGISTRY SUB=L44 CSS FUL L39

100.0% PROCESSED 75 ITERATIONS 17 ANSWERS

SEARCH TIME: 00.00.01

=> d sta que 157 L21 ST



VAR G1=13/14 NODE ATTRIBUTES:

NSPEC IS RC AT 11

CONNECT IS E2 RC AT 8

CONNECT IS E2 RC AT 9

CONNECT IS E1 RC AT 13

CONNECT IS E1 RC AT 14

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

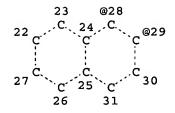
GRAPH ATTRIBUTES:

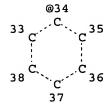
RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L23 241180 SEA FILE=REGISTRY SSS FUL L21

L52 STR





VAR G1=O/S
VAR G2=28/29/34
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 7
CONNECT IS E2 RC AT 8
CONNECT IS E2 RC AT 9
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 22, 16 33 NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

L54 16576 SEA FILE=REGISTRY SUB=L23 SSS FUL L52 L55 STR

VAR G1=O/S
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 33
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 32
GGCAT IS MCY UNS AT 33
DEFAULT ECLEVEL IS LIMITED

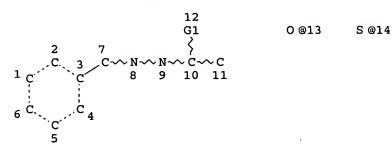
GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE L57 328 SEA FILE=REGISTRY SUB=L54 CSS FUL L55

100.0% PROCESSED 16576 ITERATIONS SEARCH TIME: 00.00.02

328 ANSWERS

=> d sta que 169 L21 STR



VAR G1=13/14

NODE ATTRIBUTES:

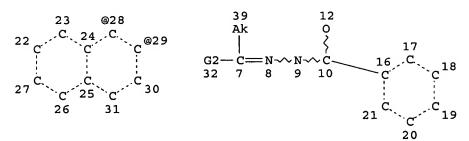
NSPEC IS RC AT 11
CONNECT IS E2 RC AT 8
CONNECT IS E2 RC AT 9
CONNECT IS E1 RC AT 13
CONNECT IS E1 RC AT 14
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

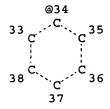
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L23 241180 SEA FILE=REGISTRY SSS FUL L21 L62 STR





VAR G2=28/29/34

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 8

CONNECT IS E2 RC AT 9 CONNECT IS E1 RC AT 12

CONNECT IS E1 RC AT 39

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 22 33 16 NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L64 9945 SEA FILE=REGISTRY SUB=L23 SSS FUL L62 L65 STR

VAR G1=H/AK
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 32
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 32
GGCAT IS MCY UNS AT 40
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L67 494 SEA FILE=REGISTRY SUB=L64 CSS FUL L65 L68 STR

40 41

39 12
Ak 0

|
Cb-C=N~N-C-Cb-Ak

NODE ATTRIBUTES:

32 7 8 9 10

CONNECT IS M1 RC AT 32
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 32
GGCAT IS MCY UNS AT 40
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L69 378 SEA FILE=REGISTRY SUB=L67 CSS FUL L68

100.0% PROCESSED 494 ITERATIONS SEARCH TIME: 00.00.01

378 ANSWERS

=> d sta que 178 L21 STR

VAR G1=13/14

NODE ATTRIBUTES:

NSPEC IS RC AT 11 CONNECT IS E2 RC AT 8 CONNECT IS E2 RC AT 9

CONNECT IS E1 RC AT 13 CONNECT IS E1 RC AT 14

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

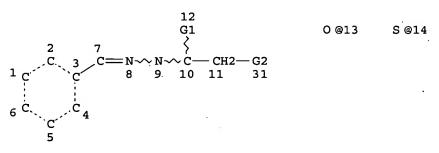
RING(S) ARE ISOLATED OR EMBEDDED

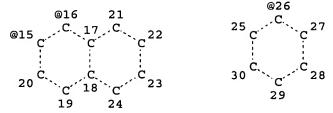
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L23 241180 SEA FILE=REGISTRY SSS FUL L21

L71 STF





VAR G1=13/14
VAR G2=16/15/26
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 8
CONNECT IS E2 RC AT 9
CONNECT IS E1 RC AT 13
CONNECT IS E1 RC AT 14
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 1 15 25

```
NUMBER OF NODES IS 31
```

STEREO ATTRIBUTES: NONE

L73 3116 SEA FILE=REGISTRY SUB=L23 SSS FUL L71

L74 STR

12 G1 \$ G2-Cb-C=N~N~C-CH2-Cb 33 32 7 8 9 10 11 31

VAR G1=O/S
VAR G2=H/X
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 31
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 31
GGCAT IS MCY UNS AT 32
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L76 127 SEA FILE=REGISTRY SUB=L73 CSS FUL L74

L77 1 SEA FILE=REGISTRY ABB=ON PLU=ON L76 AND 2 NAPHTH?

L78 126 SEA FILE=REGISTRY ABB=ON PLU=ON L76 NOT L77

=> d his

L1

(FILE 'HOME' ENTERED AT 06:44:31 ON 26 APR 2005)
DEL HIS

FILE 'HCAPLUS' ENTERED AT 06:46:29 ON 26 APR 2005

6 S (US20020173031 OR US6448472)/PN OR (US2002-047251# OR WO2000-

L2 4 S L1 NOT (KUSU ? OR BRUNELLE ?)/AU

SEL RN

FILE 'REGISTRY' ENTERED AT 06:48:54 ON 26 APR 2005

L3 51 S E1-E51

L4 20 S L3 AND SOL/FA

L5 6 S L3 AND UNSPECIFIED NOT L4

L6 25 S L3 NOT L4, L5

L7 6 S L6 AND (C13H17N3O4 OR C18H2ON2O2 OR C20H18N2O OR C19H15BRN2O

FILE 'HCAPLUS' ENTERED AT 06:51:54 ON 26 APR 2005

E THOMAS C/AU

L8 287 S E3,E18,E19

E THOMAS COLLIN/AU

L9 8 S E3-E5

E THOMAS COLIN/AU

L10 8 S E3

E WINDSOR J/AU

L11 13 S E3, E5, E6, E9

L12 1 S E13

E ROUX S/AU

L13 171 S E3, E5, E19-E22

E LLOYD A/AU

L14 33 S E3, E16, E17

L15 46 S E33, E36, E37

E HURLEY L/AU 258 S E3-E9,E13-E17 L16 FILE 'REGISTRY' ENTERED AT 06:54:10 ON 26 APR 2005 L17 STR L18 50 S L17 L19 STR L17 L20 50 S L19 L21 STR L19 L2250 S L21 L23 241180 S L21 FUL L24 . STR L25 2 S L24 CSS SAM SUB=L23 L26 STR L24 L27 0 S L26 CSS SAM SUB=L23 L28 229 S L24 CSS FUL SUB=L23 SAV TEMP L28 HANLEY047A/A L29 130 S L26 FUL SUB=L28 SAV L29 HANLEY047B/A L30 26 S L29 AND C6-C6/ES L31 24 S L30 NOT 2 NAPHTHALENE? L32 104 S L29 NOT L30 L33 · 10 S L32 AND NR>=3 6 S L33 NOT (C24H26N4O2 OR C19H24N2O2 OR C25H28N2O4) L34 94 S L32 NOT L33 L35 L36 5 S L35 AND (C19H24N2O3 OR C15H16N2O OR C15H17N3O OR C20H26N2O3 O L37 89 S L35 NOT L36 SAV L38 HANLEY047C/A DEL HANLEY047C/A L38 119 S L31, L34, L37 SAV L38 HANLEY047C/A L39 STR L24 L40 0 S L39 CSS SAM SUB=L23 50 S L39 SAM SUB=L23 L41 L42 STR L39 L43 4 S L42 SAM SUB=L23 75 S L42 FUL SUB=L23 L44 SAV L44 HANLEY047D/A L45 17 S L39 CSS FUL SUB=L44 SAV L45 HANLEY047E/A L46 58 S L44 NOT L45 L47 11 S L46 AND (C16H23N3O3 OR C20H31N3O3 OR C13H17N3O3 OR C14H19N3O3 L48 10 S L47 NOT DINITRO L49 2 S L30 NOT L31 L50 STR L21 L51 50 S L50 SAM SUB=L23 STR L50 L52 50 S L52 SAM SUB=L23 L53 16576 S L52 FUL SUB=L23 L54 SAV TEMP L54 HANLEY047F/A L55 STR L52 11 S L55 CSS SAM SUB=L54 L56 L57 328 S L55 CSS FUL SUB=L54 SAV TEMP L57 HANLEY047G/A L58 STR L55 L59 . 0 S L58 CSS SAM SUB=L57 L60 3 S L58 CSS FUL SUB=L57 SAV L60 TEMP HANLEY047H/A L61 325 S L57 NOT L60 L62 STR L50 L63 11 S L62 SAM SUB=L23 9945 S L62 FUL SUB=L23 L64

SAV TEMP L64 HANLEY047I/A

```
L65
                STR L62
L66
            32 S L65 CSS SAM SUB=L64
L67
            494 S L65 CSS FUL SUB=L64
                SAV TEMP L67 HANLEY047J/A
L68
                STR L65
L69
            378 S L68 CSS FUL SUB=L67
                SAV L69 HANLEY047K/A TEMP
L70
            116 S L67 NOT L69
L71
                STR L21
L72
            50 S L71 SAM SUB=L23
L73
           3116 S L71 FUL SUB=L23
                SAV TEMP L73 HANLEY047L/A
L74
                STR L71
              5 S L74 CSS SAM SUB=L73
L75
            127 S L74 CSS FUL SUB=L73
L76
                SAV L76 TEMP HANLEY047M/A
L77
              1 S L76 AND 2 NAPHTH?
L78
            126 S L76 NOT L77
          20779 S ?PHOSPHATASE?/CNS
L79
                DEL HANLEY047B/A
                SAV TEMP HANLEY047B/A L29
                DEL HANLEY047C/A
                SAV TEMP HANLEY047C/A L37
                DEL HANLEY047D/A
                SAV TEMP HANLEY047D/A L44
                DEL HANLEY047E/A
              SAV TEMP HANLEY047E/A L45
     FILE 'HCAOLD' ENTERED AT 07:58:27 ON 26 APR 2005
L80
             21 S L38 OR L45 OR L60 OR L61 OR L69 OR L78
     FILE 'REGISTRY' ENTERED AT 08:00:18 ON 26 APR 2005
L81
           1074 S L38, L49, L45, L48, L57, L60, L61, L69, L70, L78, L77
L82
                STR L21
L83
           1073 S L82 FUL SUB=L81
              1 S L81 NOT L83
L84
                SAV L83 TEMP HANLEY047N/A
     FILE 'HCAOLD' ENTERED AT 08:02:41 ON 26 APR 2005
L85
             20 S L83
                EDIT /AN /OREF E1-E20 /AN /OREF
     FILE 'HCAPLUS' ENTERED AT 08:03:31 ON 26 APR 2005
L86
             39 S E1-E20
                SEL DN AN 2 4 6 10 13 15 17 19 21 23 25 27 29 31 33 35 37 39
L87
             21 S L86 NOT E21-E74
L88
            123 S L83
L89
             14 S L87 AND L88
L90
              O S L89 AND (PLANT? OR AGR?)/SC,SX,CW,CT,BI .
              0 S L89 AND ?PHOSPHATASE?
L91
L92
         196912 S L79
L93
              0 S L87 AND L92
L94
              0 S L87, L89 AND (DRUG? OR PHARMACEUT? OR PHARMACOL? OR DISEAS?)
L95
             21 S L87, L89
L96
              8 S L2, L8-L16 AND L88
            101 S L88 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)
L97
             7 S L83 (L) AGR/RL
L98
             25 S L83 (L) (THU OR DMA OR PAC OR PKT OR BAC OR BUU OR DGN)/RL
             27 S L83 (L) BIOL+NT/RL
L100
L101
            38 S L83 AND (AGR? OR PHARMACEUT? OR PHARMACOL? OR PATHOL? OR IMMU
             8 S L88 AND (L92 OR ?PHOSPHATASE?)
L102
            29 S L97 AND L98-L102
L103
```

```
34 S L96, L103
L104
L105
           12 S L88 AND (PLANT? OR AGR?)/SC, SX, CW, CT, BI
L106
             8 S L105 AND L97
L107
             35 S L104,L106
                E DRUG RESISTANCE/CT
L108
         25966 S E3-E7
          70909 S E3+OLD, NT, PFT, RT
             4 S L88 AND L108, L109
L110
              2 S L110 AND L97
L111
             35 S L107, L111
L112
                E TRANSPORT PROTEIN/CT
L113
          2466 S E63-E71
        407311 S E59+OLD, NT, PFT, RT
L114
             6 S L88 AND L113,L114
L115
             3 S L115 AND L97
L116
L117
             35 S L112, L116
             6 S L88 AND ABC?
L118
L119
             6 S L118 AND TRANSPORT? (S) PROTEIN
L120
             3 S L118,L119 AND L97
            35 S L117, L120
L121
            10 S L97 AND P/DT
L122
            10 S L88 AND (?HERBIC? OR ?INSECT? OR WEED?)
L123
L124
             6 S L123 AND L97
             42 S L121, L122, L124 AND L1, L2, L8-L16, L86-L124
L125
                SEL DN AN 19 28
             40 S L125 NOT E1-E6
L126
             66 S L97 NOT L126
L127
                SEL DN AN 9 16 18 20 22 23 26 27 29 37 39 40 43 49-53 64
L128
            19 S L127 AND E7-E63
L129
             5 S L88 AND ENZYM?/SC,SX,CW,CT,BI
L130
             3 S L97 AND L129
             61 S L125, L130, L128 AND L1, L2, L8-L16, L86-L130
L131
L132
            53 S L131 NOT L96
                SEL DN AN 12 22 26
L133
           50 S L132 NOT E64-E72
             8 S L131 NOT L132
L134
           58 S L133,L134
L135
             2 S L97 AND (BIOCHEM? (L) METHOD?) /SC, SX
L136
            23 S L97 AND (BIOCHEM? OR GENETIC?)/SC,SX
L137
L138
            61 S L135-L137
L139
            11 S L138 AND (AGR? OR PLANT?)/SC,SX,CW,CT,OBI,BI
L140
             7 S L138 AND L92
L141
             8 S L138 AND ?PHOSPHATASE?
L142
             5 S L138 AND ENZYM?/SC,SX,CW,CT,BI,OBI
             8 S L138 AND L8-L16, L1, L2
L143
L144
            14 S L139-L143
            10 S L138 AND (?PARASIT? OR ?INSECT? OR ?HERBIC? OR WEED?)
L145
            16 S L144, L145
L146
           45 S L138 NOT L146
L147
            45 S L97 NOT L146, L147
L148
                SAV TEMP L87 HANLEY0470/A
                SEL HIT RN L146
                SEL HIT RN L147
     FILE 'REGISTRY' ENTERED AT 08:48:07 ON 26 APR 2005
            24 S E73-E96
1.149
L150
             61 S E97-E157
             6 S L149 AND L79
L151
             18 S L149 NOT L151
L152
L153
             57 S L150 NOT L149
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FILE 'REGISTRY' ENTERED AT 08:49:31 ON 26 APR 2005

hanley - 10 / 047251 => d ide can tot 1151 L151 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN 37289-25-1 REGISTRY RN ED Entered STN: 16 Nov 1984 Pyrophosphatase, adenosine triphosphate (9CI) (CA INDEX NAME) CN OTHER NAMES: CN Adenosine triphosphate pyrophosphatase ATP pyrophosphatase CNATP pyrophosphohydrolase CNCNAutotaxin Autotaxin-t CNE.C. 3.6.1.8 CNCN Nucleotide pyrophosphatase MF Unspecified CI MAN AGRICOLA, ANABSTR, BIOSIS, BIOTECHNO, CA, CABA, CAPLUS, LCSTN Files: EMBASE, TOXCENTER, USPATFULL *** STRUCTURE DIAGRAM IS NOT AVAILABLE *** 138 REFERENCES IN FILE CA (1907 TO DATE) 138 REFERENCES IN FILE CAPLUS (1907 TO DATE) 1: 142:295965 REFERENCE REFERENCE 2: 142:277305 REFERENCE 3: 142:173772 REFERENCE 4: 142:130156 REFERENCE 5: 142:53621 REFERENCE 6: 141:377983 REFERENCE 7: 141:363596 REFERENCE 8: 141:363589 REFERENCE 9: 141:347542 REFERENCE 10: 141:328975 L151 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN RN 9032-64-8 REGISTRY ED Entered STN: 16 Nov 1984 Pyrophosphatase, nucleotide (9CI) (CA INDEX NAME) OTHER NAMES: CN Autotaxin CN Autotaxin-t CN E.C. 3.6.1.9 CN Nucleotide pyrophosphatase CNNucleotide pyrophosphohydrolase CN Nucleotide-sugar pyrophosphatase MF Unspecified CI MAN LC AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAPLUS, CHEMCATS, EMBASE, NAPRALERT, TOXCENTER, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

357 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

357 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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142:295965
REFERENCE
            1:
REFERENCE
                142:277305
            2:
REFERENCE
            3:
                142:233710
                142:173772
REFERENCE
REFERENCE
            5:
                142:149383
REFERENCE
                142:130156
            6:
REFERENCE
            7:
                142:72870
REFERENCE
            8:
                142:53621
REFERENCE
            9:
                142:726
REFERENCE 10:
                141:377983
L151 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
     9013-05-2 REGISTRY
ED
     Entered STN: 16 Nov 1984
     Phosphatase (9CI) (CA INDEX NAME)
CN
OTHER NAMES:
CN
     4-Methylumbelliferyl phosphatase
CN
     Alkyl phosphomonoesterase
     Naphthol-AS-B1-phosphohydrolase
CN
CN
     Naphthol-AS-Bi-phosphohydrolase
CN
     Phosphoesterase
CN
     Phosphohydrolase
CN
     Phosphomonoesterase
CN
     Phosphoric acid esterase
DR
     9013-13-2
MF
    Unspecified
CI
     MAN
LC
     STN Files:
                  ADISNEWS, AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO,
       CA, CAPLUS, CASREACT, CBNB, CEN, CHEMLIST, CIN, CSCHEM, CSNB, EMBASE,
       IFICDB, IFIPAT, IFIUDB, MEDLINE, NAPRALERT, NIOSHTIC, PIRA, PROMT,
       TOXCENTER, USPAT2, USPATFULL
     Other Sources:
                      EINECS**
         (**Enter CHEMLIST File for up-to-date regulatory information)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
           14279 REFERENCES IN FILE CA (1907 TO DATE)
              64 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
           14286 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE
            1: 142:341013
REFERENCE
            2:
                142:331855
REFERENCE
            3:
                142:312728
REFERENCE
            4:
                142:311131
REFERENCE
            5:
                142:310912
REFERENCE
            6:
                142:309917
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REFERENCE

7:

142:309857

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REFERENCE
           8: 142:294490
REFERENCE
           9: 142:292732
REFERENCE 10: 142:292520
L151 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
   9001-78-9 REGISTRY
    Entered STN: 16 Nov 1984
    Phosphatase, alkaline (9CI) (CA INDEX NAME)
OTHER NAMES:
CN
    AIP
CN
    Alkaline phenyl phosphatase
    alkaline phosphatase
CN
    Alkaline phosphatase
CN
CN
    Alkaline phosphohydrolase
    Alkaline phosphomonoesterase
CN
CN
    E.C. 3.1.3.1
CN
    Ostase
    Unspecified
MF
CI
    MAN
LC
    STN Files: ADISNEWS, AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO,
      CA, CABA, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST,
      CIN, CSCHEM, CSNB, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE,
      MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA, PROMT, TOXCENTER, ULIDAT, USPAT2,
      USPATFULL
                     EINECS**, TSCA**
    Other Sources:
         (**Enter CHEMLIST File for up-to-date regulatory information)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
          35047 REFERENCES IN FILE CA (1907 TO DATE)
           1203 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
          35090 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE
          1: 142:341820
REFERENCE
           2: 142:341812
REFERENCE
           3: 142:341797
REFERENCE
           4: 142:341791
REFERENCE
           5: 142:341749
REFERENCE
           6: 142:341738
REFERENCE
           7: 142:341727
REFERENCE
           8: 142:335628
REFERENCE
           9: 142:335553
REFERENCE 10: 142:335530
L151 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
   9001-77-8 REGISTRY
    Entered STN: 16 Nov 1984
   Phosphatase, acid (9CI) (CA INDEX NAME)
OTHER NAMES:
```

CN

Acid monophosphatase

```
CN
     Acid phosphatase
CN
     Acid phosphohydrolase
     Acid phosphomonoester hydrolase
CN
     Acid phosphomonoesterase
CN
     E.C. 3.1.3.2
CN
CN ·
     Finase AP
CN
     Sumizyme PM-L
     Tartaric acid-resistant phosphatase
CN
CN
     Tartrate-resistant acid phosphatase
CN
     Tartrate-resistant phosphatase
CN
     Transferrins, uteroferrins
CN
     TRAP phosphatase
CN
     Uteroferrin
CN
     Uterotransferrins, complexes
MF
     Unspecified
CI
     MAN
LC
     STN Files: ADISNEWS, AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO,
       CA, CABA, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN,
       CSCHEM, CSNB, DDFU, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE,
       NAPRALERT, NIOSHTIC, PIRA, PROMT, TOXCENTER, ULIDAT, USPAT2, USPATFULL
     Other Sources:
                      EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
           19874 REFERENCES IN FILE CA (1907 TO DATE)
             143 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
           19888 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE
            1: 142:341788
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            2: 142:335035
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            3: 142:334951
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            4:
                142:334567
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            5:
                142:333439
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            6:
                142:333345
REFERENCE
            7:
                142:332993
REFERENCE
            8:
                142:331698
REFERENCE
            9:
                142:330615
REFERENCE 10: 142:330222
L151 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
     9000-83-3 REGISTRY
ED
     Entered STN: 16 Nov 1984
    Phosphatase, adenosine tri- (9CI) (CA INDEX NAME)
OTHER NAMES:
    Adenosine 5'-triphosphatase
CN
     Adenosine triphosphatase
CN
    ATP hydrolase
CN
    ATP phosphohydrolase
CN
CN
     Complex V (mitochondrial electron transport)
```

CN

E.C. 3.6.1.3

```
CN Uncoating ATPase
```

CN Vacuolar ATPase

DR 9013-41-6, 9016-15-3, 9036-48-0

MF Unspecified

CI MAN

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMLIST, CIN, EMBASE, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, NAPRALERT, NIOSHTIC, PROMT, TOXCENTER, USPAT2, USPATFULL

Other Sources: TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

64313 REFERENCES IN FILE CA (1907 TO DATE)
249 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
64366 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:341831

REFERENCE 2: 142:336518

REFERENCE 3: 142:336517

REFERENCE 4: 142:335218

REFERENCE 5: 142:334076

REFERENCE 6: 142:333605

REFERENCE 7: 142:333377

REFERENCE 8: 142:333286

REFERENCE 9: 142:333259

REFERENCE 10: 142:333243

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:50:35 ON 26 APR 2005
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This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> d l146 all hitstr tot
L146 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
    2005:141200 HCAPLUS
DN
    142:254568
ED
    Entered STN: 18 Feb 2005
ΤI
    Methods and compositions for increasing the efficacy of
    biologically-active ingredients such as antitumor agents
IN
    Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan
    M.; Thomas, Collin E.
    Board of Regents, the University of Texas System, USA
PA
    PCT Int. Appl., 243 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
IC
     ICM C12N
CC
     1-6 (Pharmacology)
FAN.CNT 1
    PATENT NO.
                      KIND DATE
                                         APPLICATION NO.
     -----
                       ----
                              -----
                                          -----
    WO 2005014777
                        A2
                              20050217
                                       WO 2003-US32667
PΙ
                                                               20031016
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
            GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
            LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
            OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
            TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI US 2002-418803P
                         P
                               20021016
CLASS
PATENT NO.
              CLASS PATENT FAMILY CLASSIFICATION CODES
 ------
WO 2005014777 ICM
                       C12N
    The invention provides methods and compns. for modulating the sensitivity
    of cells to cytotoxic compds. and other active agents. In accordance with
    the invention, compns. are provided comprising combinations of
    ectophosphatase inhibitors and active agents. Active agents
    include antibiotics, fungicides, herbicides,
    insecticides, chemotherapeutic agents, and plant growth
    regulators. By increasing the efficacy of active agents, the invention
    allows use of compns. with lowered concns. of active ingredients.
    antibiotic fungicide herbicide insecticide
ST
    plant growth regulator combination antitumor
IT
    Trichoderma polysporum
        ((ATCC 20475; methods and compns. for increasing the efficacy of
       biol.-active ingredients such as antitumor agents)
TT
    Trichoderma harzianum
        ((ATCC 20476); methods and compns. for increasing the efficacy of
       biol.-active ingredients such as antitumor agents)
ΙT
    Pseudomonas fluorescens
        (1629RS; methods and compns. for increasing the efficacy of
       biol.-active ingredients such as antitumor agents)
IT
    Pseudomonas fluorescens
        (A506; methods and compns. for increasing the efficacy of biol.-active
       ingredients such as antitumor agents)
ΙT
    Zeolites (synthetic), biological studies
```

Zeolites (synthetic), biological studies

```
Zeolites (synthetic), biological studies
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (Ag; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Surfactants
        (Alkanolamide; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (Bacillus thuringiensis Cry1F and Cfy1Ab; methods and compns. for
        increasing the efficacy of biol.-active ingredients such as antitumor
        agents)
IT
    Balsams
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (Canadian; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Alcohols, biological studies
    Alcohols, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (C11-15-secondary, ethoxylated; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Isoalkanes
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (C12-14; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Alcohols, biological studies
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (C12-15; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Alcohols, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (C6-12; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
    Diglycerides
    Glycerides, biological studies
    Monoglycerides
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (C8-10 monoglycerides and diglycerides; methods and compns. for
        increasing the efficacy of biol.-active ingredients such as antitumor
        agents)
    Alcohols, biological studies
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (C8-10; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
    Pseudomonas fluorescens
        (EG-1053; methods and compns. for increasing the efficacy of
       biol.-active ingredients such as antitumor agents)
IT
    Bacillus subtilis
        (GBO3; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
    Pheromones, animal
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (German cockroach; methods and compns. for increasing the efficacy of
```

```
biol.-active ingredients such as antitumor agents)
     Fats and Glyceridic oils, biological studies
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (Japan wax; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
        (Kaposi's; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Paraffin oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (Low mol. weight; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Bacillus subtilis
IT
        (MBI 600; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Gene, animal
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (MDR, Arabidopsis thaliana; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (Melaleuca alternifolia; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (Peru; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Bacillus subtilis
IT
        (QST 713 strain; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Named reagents and solutions
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (Stoddard; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Paecilomyces lilacinus
        (Strain 251; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Lymphoproliferative disorders
        (Waldenstrom's macroglobulinemia; methods and compns. for increasing
        the efficacy of biol.-active ingredients such as antitumor agents)
ΙT
     Kidney, neoplasm
        (Wilms'; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Leukemia
        (acute lymphocytic; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (adhesives; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Immunostimulants
        (adjuvants; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Silica gel, biological studies
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
```

(aerogel; methods and compns. for increasing the efficacy of

```
biol.-active ingredients such as antitumor agents)
    Flours and Meals
TT
        (alfalfa; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Amines, biological studies
IT
    Amines, biological studies
     Petroleum resins
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (aliphatic; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Delphinium
        (alkaloid; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
ΙT
    Helleborus
     Schoenocaulon
        (alkaloids; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Quaternary ammonium compounds, biological studies
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (alkylbenzyldimethyl, chlorides; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
ΙT
     Quaternary ammonium compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (alkyltrimethyl, bromides; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Quaternary ammonium compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (alkyltrimethyl, chlorides; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
ΙT
     Glycosides
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (amino; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
ΙT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (anise; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Antitumor agents
IT
        (antibiotic; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Cytotoxic agents
        (antimetabolites; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Antibiotics
       Drug resistance
        (antitumor; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
TT
     Paecilomyces fumoso-roseus
        (apopka strain 97; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Petroleum, biological studies
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (aromatic, alkylated; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
```

(barley; methods and compns. for increasing the efficacy of

```
biol.-active ingredients such as antitumor agents)
IT.
     Quaternary ammonium compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite;
        methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Quaternary ammonium compounds, biological studies
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (benzyl-C12-14-alkyldimethyl; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
ΙT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (bergamot; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Prunus amygdalus
IT
        (bitter almond; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
        (blast-furnace; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Linseed oil
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (boiled; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Essential oils
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (cade; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (cajuput; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
TΤ
     Caseins, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (calcium complexes; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IΤ
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (camphor; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Gelatins, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (capsules; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Head, neoplasm
        (carcinoma; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Milk substitutes
        (cattle; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
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(cedar leaf; methods and compns. for increasing the efficacy of

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biol.-active ingredients such as antitumor agents)
IT
     Essential oils
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (cedarwood; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Uterus, neoplasm
IT
        (cervix; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (chamomile; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Perfumes
        (cherry fragrance oil 493; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
     Paraffin waxes, biological studies
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (chloro; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Carcinoma
     Chorion, neoplasm
        (choriocarcinoma; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Leukemia
        (chronic lymphocytic; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
IT
        (chronic myelocytic; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (cinnamon; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
TT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (citronella; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Cellulose pulp
        (citrus; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (citrus; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (clove; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Naphtha
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (coal; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Amines, biological studies
·IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
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(Biological study); USES (Uses)
        (coco alkyl, compds. with tetrachlorophenol (1:1); methods and compns.
        for increasing the efficacy of biol.-active ingredients such as
        antitumor agents)
     Amides, biological studies
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (coco, N-(hydroxyethyl); methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Fatty acids, biological studies
     Fatty acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (coco, cadmium salts; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
IT
     Intestine, neoplasm
        (colon; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Bentonite, biological studies
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (compound with dimethyldioctadecylammonium chlorid; methods and compns.
        for increasing the efficacy of biol .- active ingredients such as
        antitumor agents)
     Naphthenic acids, biological studies
     Naphthenic acids, biological studies
     Resin acids
     Resin acids
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (copper salts; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Food analysis
        (corn-containing, hydrolyzed; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Flours and Meals
        (corn; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Flours and Meals
        (cottonseed; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Avena sativa
     Triticum aestivum
        (cracked; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
        (crumb; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Syzygium aromaticum
        (crushed; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
ΙT
     Isoalkanes
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (c11-12; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Quaternary ammonium compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (dicoco alkyldimethyl, chlorides; methods and compns. for increasing
        the efficacy of biol.-active ingredients such as antitumor agents)
     Fatty acids, biological studies
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
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(Biological study); USES (Uses) (dimer acids; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IΤ Urogenital tract (disease; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (distillate, heavy oils; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Coal tar RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (distillate, upper; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) ΙT Petroleum products (distillates, C12-30-aromatic; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Petroleum products (distillates, aliphatic; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Petroleum products (distillates, aromatic; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Petroleum products IT (distillates, refined; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Petroleum products (distillates; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Lime (chemical) IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (dolomitic; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT (dried; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) High throughput screening TT (drug; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Nicotiana tabacum (dust; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Uterus, neoplasm (endometrium, adenocarcinoma; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Linseed oil RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (epoxidized; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Myeloproliferative disorders (essential thrombocythemia; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Fatty acids, biological studies IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (esters; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Monoglycerides

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

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(Biological study); USES (Uses)
        (ethoxylated coco; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Lanolin
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (ethoxylated, acetate; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
IT
     Lanolin
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (ethoxylated; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (eucalyptus; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Allium cepa
     Glycine max
     Juniperus communis
     Malt
     Myrica cerifera
        (extract; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Lonchocarpus
        (exts.; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Alcohols, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (fatty; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Fats and Glyceridic oils, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (fish; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
TΤ
     Cottonseed
     Glycine max
     Secale cereale
     Zea mays
        (flour and meal; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Juglans regia
     Wood
        (flour; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Polyesters, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (foam, UL-94 HF1 listed; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
ÌТ
     Mycosis
        (fungoides; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Repellents
        (game; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Disease, animal
        (genitourinary; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
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IT

Essential oils

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (geranium; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Vitis vinifera (grape pomace; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Pseudotsuga menziesii IT (ground bark; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT (ground cobs; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Oryza sativa (ground hulls; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Sesamum indicum (ground plant; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Avena sativa (ground; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Leukemia (hairy-cell; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT (hard, oil; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Carcinoma (head; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Naphtha RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (heavy aromatic; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Petroleum, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (heavy paraffinic distillate; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Drug screening (high throughput; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Coal tar pitch (high-temperature; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Glycine max IT (hulls; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) ITNeoplasm (humoral hypercalcemia of malignancy; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT Resin acids RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (hydrogenated, Me esters; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Castor oil IT Soybean oil RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(hydrogenated; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Syrups (sweetening agents) (hydrolyzed starch; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Paraffin waxes, biological studies IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (hydrotreated; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Pancreatic islet of Langerhans, neoplasm (insulinoma; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT Syrups (sweetening agents) (invert; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Antibacterial agents (iodophors; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Pigments, nonbiological (iron oxide; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Bacillus subtilis (isolate B246; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT Ampelomyces quisqualis (isolate M-10; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Essential oils RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (jasmine; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Paints (latex; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Essential oils RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (lavender; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT Naphthenic acids, biological studies Naphthenic acids, biological studies Naphthenic acids, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (lead salts; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Eucalyptus Mentha pulegium (leaves; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT Essential oils RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (lemon; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Essential oils IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (lemongrass; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT

Skin, disease

(lesion; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Essential oils RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (lime; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Capsicum annuum annuum (longum group, paprika; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Beta vulgaris saccharifera Fish Meat Medicago sativa (meal; methods and compns. for increasing the efficacy of biol .- active ingredients such as antitumor agents) IT Flours and Meals (meat meal; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Fats and Glyceridic oils, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (menhaden; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Naphthenic acids, biological studies Naphthenic acids, biological studies Naphthenic acids, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (mercury salts; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT. Acacia Adrenal cortex, neoplasm Agrobacterium tumefaciens Agrobacterium vitis Agrotis segetum granulovirus Alkylating agents, biological Allium cepa Allium sativum Ampelomyces quisqualis Anthracene oil Antibiotic resistance Arabidopsis thaliana Arachis hypogaea Aschersonia alevrodis Avena sativa Bacillus sphaericus Bacillus thuringiensis Beeswax Bladder, neoplasm Bone meal Brain, neoplasm Bran Capsicum Caramel (color) Carcinoid Chamomile Cheese Cinnamon (horticultural common name) Combination chemotherapy Cork Corncob

Cottonseed meal

Creosote Cytotoxic agents Daucus carota Desmodium Drug delivery systems Drug screening Drugs Esophagus, neoplasm Fumigants Fungicides Gentiana Glues Glues Gossypium hirsutum Herbicides Hodgkin's disease Honey Human Insecticides Jet aircraft fuel Liliopsida Lung, neoplasm Magnoliopsida Mammary gland, neoplasm Meat Medicago sativa Melanoma Mentha piperita Milk Mint Molasses Multiple myeloma Nicotiana tabacum Nucleopolyhedrovirus Oatmeal Odor and Odorous substances Oryza sativa Ovary, neoplasm Paenibacillus popilliae Paints Paper Paperboard Peanut butter Phlebia gigantea Phlebiopsis gigantea Polycythemia vera Prostate gland, neoplasm Pseudomonas chlororaphis Puccinia canaliculata Quassia Quillaja Rabbit calicivirus Raisin Repellents Rosmarinus officinalis Sawdust Seaweed Sinorhizobium meliloti Skin, neoplasm Solanum tuberosum Solvent naphtha Solvent naphtha

Solvent naphtha

Solvent naphtha Sorghum bicolor Sphagnum Staphylococcus aureus Stomach, neoplasm Testis, neoplasm Theobroma cacao Theobroma cacao Thickening agents Thymus (plant) Tomato mosaic virus Trigonella foenum-graecum Triticum aestivum Verticillium lecanii Wheat flour Wheat flour Whey Wool Yeast Zea mays (methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Amino acids, biological studies Androgens Asbestos Asphalt Bentonite, biological studies Canola oil Carbon black, biological studies Caseins, biological studies Castor oil Chlorinated natural rubber Coal tar Coal tar Coal tar Coconut oil Cod liver oil Collagens, biological studies Corn oil Corticosteroids, biological studies Cottonseed oil Creosote oil Cytokinins Diatomite Epoxy resins, biological studies Essential oils Feldspar-group minerals Fertilizers Gasoline Gelatins, biological studies Gibberellins Glycopeptides Granite, biological studies Growth regulators, plant Humic acids Hydrocarbon oils Hydrocarbon oils Jojoba oil Kaolin, biological studies Kerosene Lard Ligroine Lime (chemical)

Linseed oil Macrolides Mica-group minerals, biological studies Naphthenic acids, biological studies Naphthenic oils Natural products, pharmaceutical Nitrile rubber, biological studies Olive oil Palm oil Paraffin oils Paraffin oils Paraffin waxes, biological studies Peanut oil Perlite Petrolatum Petroleum hydrocarbons Petroleum resins Petroleum spirits Phenols, biological studies Phosphoproteins Plastics, biological studies Polyamides, biological studies Polyamides, biological studies Polyamines Polyenes Polyoxyalkylenes, biological studies Polysiloxanes, biological studies Polysiloxanes, biological studies Polysiloxanes, biological studies Polyurethanes, biological studies Polyvinyl butyrals Progestogens Protein hydrolyzates Pumice Pyrethrins Pyrethrins Pyrethrins Pyrethrins Rape oil Resins Rosin Rubber, biological studies Safflower oil Sand Saponins Shale Shellac Silica gel, biological studies Soaps Soapstone Soybean oil Tall oil Tallow Tetracyclines Tung oil Turpentine Waxes Wood tar Zeins RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

Fats and Glyceridic oils, biological studies IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (mink; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Anagrapha falcifera (multi-nuclear polyhedrosis virus (AFMNPV); methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Skin, neoplasm IT (mycosis fungoides; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT (neck; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT (needle oil; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Neck, anatomical (neoplasm, carcinoma; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Nerve, neoplasm (neuroblastoma; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Chloramines RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (nitrogen mustards; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Fuel oil (number 1; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Diesel fuel Fuel oil (number 2; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Fuel oil (number 4; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Fuel oil (number 6; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT (non-Hodgkin's; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Surfactants (nonionic; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Alkanes, biological studies IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (normal C5-20; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Neodiprion sertifer (nuclear polyhedrosis virus; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Aloe barbadensis Lavandula hybrida (oil; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Resins

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

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(oleoresins, capsicum; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
IT
     Bone, neoplasm
     Sarcoma
        (osteosarcoma; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (partially hydrogenated; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Citrus limon
        (peel oil; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
TT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (pepper, Piper nigrum berry; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (peppermint; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
TT
     Sulfonic acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (petroleum, sodium salts; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT . Tar
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (pine, oil; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Essential oils
     Tar
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (pine; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
TT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (polymerized; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Vinyl compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (polymers, synthetic; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
TT
    Vinyl compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (polymers; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Malus pumila
        (pomace; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
        (poultry; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Gelatins, biological studies
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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses) (powdered; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Beta vulgaris (powder; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT (product, hydrolyzed; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Carcinoma IT (pulmonary small-cell; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Citrus sinensis TΤ (pulp; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TΤ Xanthomonas campestris (pv Poannua; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Antitumor agents (resistance to; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Sarcoma (rhabdomyosarcoma; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Essential oils TΤ RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (rosemary; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) ITEssential oils RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (rosin; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Flours and Meals IT (rye; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Naphthenic acids, biological studies IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (salts, compound with dodecyldimethylbenzylammonium; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Sulfonic acids, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (salts; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT Essential oils RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sassafras; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT (scraps; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT (seed oil; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT (seed; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

Bacillus sphaericus

TT

(serotype H-5A5B, strain 2362; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Fats and Glyceridic oils, biological studies IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sesame; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Fertilizers RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sewage sludge; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Egg (shell; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Juglans regia (shells, ground; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Arachis hypogaea (shells; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Lung, neoplasm IT (small-cell carcinoma; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Caseins, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sodium complexes; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Polyphosphoric acids Sulfonic acids, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sodium salts; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TΤ RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sodium tallow; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Animal tissue, disease (soft, neoplasm, sarcoma; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Sarcoma (soft-tissue; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Amines, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (soya alkyl, ethoxylated; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Fatty acids, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (soya, Me esters; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Flours and Meals IT (soybean; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Proteins IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(soybean; methods and compns. for increasing the efficacy of

biol.-active ingredients such as antitumor agents) Essential oils TТ RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (spearmint; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Fats and Glyceridic oils, biological studies IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sperm oil; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Phlebiopsis gigantea (spores and mycelium spores; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Gliocladium catenulatum Nosema locustae Paenibacillus popilliae (spores; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Pseudomonas chlororaphis (strain 63-28; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Pseudomonas syringae (strain 742 RS; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Pseudomonas syringae (strain AGS31 & strain PS31; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Bacillus cereus (strain BPO; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Pseudomonas syringae IT (strain ESC-10; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Pseudomonas syringae (strain ESC-11; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Agrobacterium tumefaciens IT (strain K1026; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Streptomyces griseoviridis (strain K61; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Agrobacterium tumefaciens IT (strain K84; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Pseudomonas fluorescens (strain NCIB 12089; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT Pseudomonas chlororaphis (strain Tx-1; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Bacillus cereus (strain UW85; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Hordeum vulgare (straw; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Bacillus thuringiensis IT (sub Kurstaki strain EG7673 coleopteran active toxin; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

Bacillus thuringiensis

IT

(sub Kurstaki strain EG7673 lepidopteran active toxin; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Aizawai, GC-91 protein; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Aizawai, serotype H-7; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Aizawai; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Israelensis, serotype H-14; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Kurstaki strain SA-12; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Kurstaki, genetically engineered strain AGRO1 by Agrevo; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Kurstaki, genetically engineered strain AGRO2 by Agrevo; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Kurstaki, serotype; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Kurstaki, strain EG2348; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Kurstaki, strain EG2371; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Kurstaki, strain EG2424; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp.Kurstaki, strain SA-1 1; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Morrisoni, serotype 8a8b; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

Bacillus thuringiensis

(subsp San Diego; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subsp Tenebrionis; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subspec Tenebrionis delta endotoxin; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subspecies Israelensis strain EG2215; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis

(subspecies Israelensis, strain IPS-78; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Bacillus thuringiensis (subspecies Kurstaki strain HD-1, lepidopteran active toxin; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Bacillus thuringiensis IT (subspecies kurstaki strain BMP 123; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Bacillus thuringiensis IT (subspecies kurstaki, genetically engineered strain EG7841 lepidopteran active toxin; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Cod liver oil RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sulfonated; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Petroleum, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sulfurized; methods and compns. for increasing the efficacy of biol -active ingredients such as antitumor agents) IT Helianthus annuus (sunflower seed; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT (sunflower; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Fatty acids, biological studies Fatty acids, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (tall-oil, copper salts; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT Fatty acids, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (tall-oil; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Essential oils RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (thyme, Thymus vulgaris; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Burkholderia cepacia (type Wisconsin; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) ITPetroleum, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (unrefined; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Carcinoma (uterine endometrial adenocarcinoma; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Bacillus thuringiensis (var Kurstaki strain M-200 protein toxin; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Bacillus thuringiensis (var Kurstaki, genetically engineered strain ECX; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

Bacillus thuringiensis

IT

(var Kurstaki, genetically engineered strain EG7826 Lepidopteran active toxin; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Bacillus thuringiensis (var kurstaki delta endotoxin protein; methods and compns. for increasing the efficacy of biol .- active ingredients such as antitumor agents) Fats and Glyceridic oils, biological studies TΤ RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (vegetable, hydrogenated; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Fats and Glyceridic oils, biological studies TT Fats and Glyceridic oils, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (vegetable; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Alkaloids, biological studies IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (vinca; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Dyes (water-soluble; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Glycerides, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (wheat germ-oil; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Fats and Glyceridic oils, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (wheat germ; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT Pepper (spice) (white; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) ΙT Essential oils RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (wintergreen; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Linseed oil RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (with driers; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Creosote (wood; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Naphthenic acids, biological studies IT Naphthenic acids, biological studies Resin acids Resin acids RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (zinc salts; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) TT Interferons

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

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(\alpha; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Lactams
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (\beta-; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
ΙT
     74-82-8D, Methane, triaryl derivs.
                                        85-86-9, Sudan III
                                                                109-76-2D,
     1,3-Propanediamine, N-alkyl derivs., salts
                                                 115-31-1, Thanite
     814-49-3
                2439-00-1
                            3032-40-4
                                        3397-62-4
                                                    3768-14-7
                                                                 4147-57-3
     7206-15-7
                 7206-27-1
                             8003-06-3
                                         8003-19-8D, derivs.
                                                               8064-49-1, Tenox
         8066-01-1
                     8076-84-4, Tenox 4
                                          9003-01-4
                                                       9003-05-8, Polyacrylamide
     11144-43-7
                  12770-24-0, Toximul-P
                                          26532-25-2
                                                       31895-21-3, Thiocyclam
     35513-93-0D, N-C6-18alkyl derivs.
                                         37300-16-6, Versalon 1112
                                                                      37350-66-6
     39384-60-6, Tenox S 1 41481-51-0
                                          50863-22-4
                                                       51068-60-1, Sulglycapin
     51796-19-1, Thixatrol ST
                                51811-79-1, T-Mulz 565
                                                         52236-30-3
     52508-35-7
                 58175-59-0
                               58175-60-3
                                            60864-33-7, Triton CF-10
                              63100-33-4, Triton X 363
                                                         66227-09-6
     62031-70-3, Wingstay V
     67053-55-8, Toximul D
                             70193-21-4, Trichlamide
                                                       72459-58-6, Triazoxide
     76608-88-3, Triapenthenol
                                 76930-44-4, Po-san A
                                                        81412-43-3, Tridemorph
     83869-01-6, TF 310
                          85411-41-2, T-Mulz AO 2
                                                   87917-06-4, Tensiofix B
     7416
            87917-07-5, Tensiofix B 7453
                                          92302-40-4
                                                        92529-51-6, Sure-Sol
           94189-31-8, Stepantan A
                                    99105-77-8, Sulcotrione
                                                               103737-35-5,
                 116170-30-0, Thicyofen
                                         118134-30-8, Spiroxamine
     119515-38-7, Propidine
                              123249-43-4, Thidiazimin
                                                         130561-48-7, Cintofen
                   154201-55-5
                                               171248-07-0
     139963-64-7
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     291536-80-6 291536-82-8 291536-84-0
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     845739-24-4
                   845739-25-5
                                 845739-26-6
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                                                              845739-28-8
     845739-29-9
     RL: PAC (Pharmacological activity); THU (Therapeutic
     use); BIOL (Biological study); USES (Uses)
        (methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     9003-18-3
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (nitrile rubber; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     11121-88-3, Versamid
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (resin binder; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
ΙT
     291536-82-8 291536-84-0 291536-87-3
     358622-53-4
     RL: PAC (Pharmacological activity); THU (Therapeutic
     use); BIOL (Biological study); USES (Uses)
        (methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
RN
     291536-82-8 HCAPLUS
CN
     1-Naphthaleneacetic acid, [(2-hydroxy-5-methylphenyl)methylene]hydrazide
           (CA INDEX NAME)
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RN 291536-84-0 HCAPLUS
CN 1-Naphthaleneacetic acid, [(4-bromophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 291536-87-3 HCAPLUS
CN Acetic acid, (2,4,6-trimethylphenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

RN 358622-53-4 HCAPLUS

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L146 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     2003:23438 HCAPLUS
DN
     138:68713
ED
     Entered STN: 10 Jan 2003
TI
     Modulating resistance of tumor and pathogen cells to foreign compounds by
     manipulation of ATP gradients via regulation of ABC transporters
     and ecto-phosphatases
IN
     Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan
PA
     University of Texas, USA
so
     U.S. Pat. Appl. Publ., 41 pp., Cont.-in-part of U.S. Ser. No. 261,825.
     CODEN: USXXCO
DT
     Patent
LA
     English
IC
     ICM C12N009-12
     ICS C12N009-00
INCL 435194000; 435183000
     6-1 (General Biochemistry)
     Section cross-reference(s): 1, 5, 7,
     10, 11, 13
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     PATENT NO.
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                                            APPLICATION NO.
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PI
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         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI US 1999-244792
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     US 1999-261825
                          A2
                                19990303 <--
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US 2002-134019
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CLASS
PATENT NO.
                CLASS PATENT FAMILY CLASSIFICATION CODES
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US 2003008369
                ICM
                ICS
                       C12N009-00
                INCL
                       435194000; 435183000
US 2003008369
                NCL
                       435/194.000; 435/183.000
                ECLA
                       A61K009/00M20B; A61K031/165+A; A61K031/165H;
                       A61K031/165P; A61K031/18; A61K031/215L; A61K031/215L10;
                       A61K031/24; A61K031/35P10; A61K031/38H; A61K031/40T10;
                       A61K031/425F; A61K038/13; A61K038/13+M; C07K014/705;
                       C12N009/14; C12N015/82C8B4
US 2002006901
                NCL
                       514/011.000; 514/009.000; 424/045.000
                ECLA
                       A61K009/00M20B; A61K038/13; A61K038/13+M
AB
     The present invention relates to methods for modulating the growth of
     tumor and pathogen cells and the resistance of cells to foreign compds.,
     i.e. drugs, antibiotics, etc. by altering the ATP gradient across biol.
    membranes. The altering of the ATP gradient across biol. membranes is
    achieved through the manipulation of ecto-phosphatase (e.g.,
    human apyrase) activity and ABC transporter mol. (e.g.,
    Arabidopsis AtPGP-1) activity which may also be useful to confer
    herbicide resistance to plants, confer antibiotic
     resistance to bacteria, confer drug resistance to yeast cells, or to
     reduce resistance in cells to facilitate chemotherapeutic treatments, and
     to reduce resistance in bacteria and yeast. The present invention is also
     directed to the methods for identifying ecto-phosphatase
     inhibitors and uses thereof. Nineteen ecto-phosphatase
     inhibitory mols. are provided which are useful in reversing multi-drug
     resistance in Arabidopsis and yeast.
    drug resistance ATP gradient ABC transporter phosphatase
     ; antibiotic resistance ATP gradient ABC transporter
    phosphatase; herbicide resistance ATP gradient
     ABC transporter phosphatase; tumor multidrug resistance
    ATP gradient modulation
IT
     Transport proteins
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (ABC (ATP-binding cassette)
        transporters; modulating resistance of tumor and pathogen cells
        to foreign compds. by manipulation of ATP gradients via regulation of
       ABC transporters and ecto-phosphatases)
IT
    Neoplasm
        (bone marrow; modulating resistance of tumor and pathogen cells to
        foreign compds. by manipulation of ATP gradients via regulation of
       ABC transporters and ecto-phosphatases)
IT
     Intestine, neoplasm
        (colon; modulating resistance of tumor and pathogen cells to foreign
        compds. by manipulation of ATP gradients via regulation of ABC
        transporters and ecto-phosphatases)
IT
     Antibiotics
     Antitumor agents
      Herbicides
        (increasing effectiveness of; modulating resistance of tumor and
       pathogen cells to foreign compds. by manipulation of ATP gradients via
       regulation of ABC transporters and ecto-phosphatases
     Antibiotic resistance
IT
    Bladder, neoplasm
     Bone, neoplasm
     Brain, neoplasm
       Drug resistance
      Herbicide resistance
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Human

Liver, neoplasm Lung, neoplasm Lymphoma Mammalia Mammary gland, neoplasm Multidrug resistance Ovary, neoplasm Pancreas, neoplasm Prostate gland, neoplasm Skin, neoplasm Staphylococcus Staphylococcus aureus Stomach, neoplasm Testis, neoplasm (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases) P-glycoproteins RL: BSU (Biological study, unclassified); BIOL (Biological study) (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases) Bone marrow, disease (neoplasm; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases) Animal tissue, disease (soft, neoplasm; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases) Neoplasm (soft-tissue; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases) 865-21-4, Vinblastine RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (increasing effectiveness of; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases 61-32-5, Methicillin RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (inhibiting growth of cells resistant to; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ectophosphatases) 154201-55-5 41481-51-0 139963-64-7 168832-50-6 171248-07-0 291536-81-7 291536-82-8 291536-79-3 291536-80-6 **291536-84-0 291536-85-1** 291536-86-2 **291536-87-3** 291536-88-4 291536-89-5 291536-90-8 291536-92-0 291536-91-9 313493-42-4 RL: AGR (Agricultural use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases) 9000-95-7, Apyrase 9013-05-2 56-65-5, 5'-ATP, biological studies Phosphatase RL: BSU (Biological study, unclassified); BIOL (Biological study) (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC

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transporters and ecto-phosphatases)

IT 291536-82-8 291536-84-0 291536-85-1
291536-87-3

RL: AGR (Agricultural use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

RN 291536-82-8 HCAPLUS

CN 1-Naphthaleneacetic acid, [(2-hydroxy-5-methylphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 291536-84-0 HCAPLUS
CN 1-Naphthaleneacetic acid, [(4-bromophenyl)methylene]hydrazide (9CI) (CAINDEX NAME)

RN

CN Benzoic acid, 3-methyl-, [1-(2-naphthalenyl)ethylidene]hydrazide (9CI) (CA INDEX NAME)

RN 291536-87-3 HCAPLUS

CN Acetic acid, (2,4,6-trimethylphenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

IT 9013-05-2, Phosphatase

RL: BSU (Biological study, unclassified); BIOL (Biological study) (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

RN 9013-05-2 HCAPLUS

CN Phosphatase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L146 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:870013 HCAPLUS

DN 138:200817

ED Entered STN: 17 Nov 2002

TI Automated colorimetric screen for apyrase inhibitors

AU Windsor, J. B.; Thomas, C.; Hurley, L.; Roux, S. J.; Lloyd, A. M.

CS The University of Texas at Austin, Austin, TX, USA

SO BioTechniques (2002), 33(5), 1024,1026,1028-1030 CODEN: BTNODO; ISSN: 0736-6205

PB Eaton Publishing Co.

DT Journal

LA English

CC 7-3 (Enzymes)

- AB Apyrases are enzymes that efficiently hydrolyze ATP and ADP and may operate both inside and outside the cell. Although apyrases are important to a variety of cellular mechanisms and uses in industry, there are no available apyrase-specific inhibitors. Colorimetric assays based on the Fiske-Subbarow method for measuring inorg. phosphate are able to detect the release of inorg. phosphate from ATP and other nucleotides. We found that this type of assay could be automated and used to screen for apyrase-inhibiting compds. by assaying for a reduction in released phosphate in the presence of potential inhibitors. The automation of this assay allowed for the successful screening of a com. available compound library. Several low mol. weight compds. were identified that, when used at micromolar concns., effectively inhibited apyrase activity.
- ST colorimetry screen apyrase inhibitor
- IT Colorimetry

Computer application

(automated colorimetric assays based on the Fiske-Subbarow method for screening for apyrase inhibitors) Hydrazones IT RL: BSU (Biological study, unclassified); BIOL (Biological study) (naphthylacetyl, derivs.; automated colorimetric assays based on the Fiske-Subbarow method for screening for apyrase inhibitors) ITEnzyme kinetics (of inhibition; automated colorimetric assays based on the Fiske-Subbarow method for screening for apyrase inhibitors) IT Imides Sulfonic acids, biological studies RL: BSU (Biological study, unclassified); BIOL (Biological study) (sulfonimides; automated colorimetric assays based on the Fiske-Subbarow method for screening for apyrase inhibitors) 56-65-5, 5'-ATP, biological studies 9000-83-3, ATPase IT 9000-95-7, Apyrase 9001-77-8, Acid phosphatase 9001-78-9, Alkaline phosphatase 9014-00-0, E.C. 1.14.14.3 29556-18-1D, derivs. 291536-84-0, NGXT 195 291536-91-9, NGXT 1913 313493-42-4, NGXT 199 RL: BSU (Biological study, unclassified); BIOL (Biological study) (automated colorimetric assays based on the Fiske-Subbarow method for screening for apyrase inhibitors) RE.CNT THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD (1) Beukers, M; Biochem Pharmacol 1993, V46, P1959 HCAPLUS (2) Bodas, E; J Biol Chem 2000, V275, P20268 HCAPLUS (3) Durward, E; BioTechniques 1998, V25, P608 HCAPLUS (4) Dzhandzhugazyan, K; FEBS Lett 1998, V430, P227 HCAPLUS (5) Fiske, C; J Biol Chem 1925, V66, P375 HCAPLUS (6) Gao, X; J Biol Chem 1999, V274, P21450 HCAPLUS (7) Gendron, F; J Med Chem 2000, V43, P2239 HCAPLUS (8) Handa, M; Biochem Biophys Res Commun 1996, V218, P916 HCAPLUS (9) Karamohamed, S; BioTechniques 2001, V31, P420 HCAPLUS (10) Kirchgesser, M; J Clin Chem Clin Biochem 1990, V28, P407 HCAPLUS (11) Knowles, A; Eur J Biochem 1999, V26, P349 (12) Ngo, H; Exp Parasitol 2000, V95, P148 HCAPLUS (13) Plesner, L; Int Rev Cytol 1995, V158, P141 HCAPLUS (14) Sakakibara, T; Anal Biochem 1997, V250, P157 HCAPLUS (15) Silverman, J; J Biol Chem 1998, V273, P12352 HCAPLUS (16) Stanley, P; ATP Luminescence: Rapid Methods in Microbiology 1989 (17) Westfall, T; Br J Pharmacol 1996, V117, P867 HCAPLUS (18) Ziganshin, A; Drug Dev Res 1994, V32, P134 HCAPLUS 9000-83-3, ATPase 9001-77-8, Acid phosphatase 9001-78-9, Alkaline phosphatase 291536-84-0, **NGXT 195** RL: BSU (Biological study, unclassified); BIOL (Biological study) (automated colorimetric assays based on the Fiske-Subbarow method for screening for apyrase inhibitors) 9000-83-3 HCAPLUS RNPhosphatase, adenosine tri- (9CI) (CA INDEX NAME) CN *** STRUCTURE DIAGRAM IS NOT AVAILABLE *** RN 9001-77-8 HCAPLUS CN Phosphatase, acid (9CI) (CA INDEX NAME) *** STRUCTURE DIAGRAM IS NOT AVAILABLE *** RN9001-78-9 HCAPLUS CN Phosphatase, alkaline (9CI) (CA INDEX NAME) *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN

291536-84-0 HCAPLUS

CN 1-Naphthaleneacetic acid, [(4-bromophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

AB

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L146 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
    2002:833490 HCAPLUS
    137:306061
DN
ED
    Entered STN: 01 Nov 2002
TΙ
    Pesticidal and herbicidal activity through modulation of animal
    and plant cell membrane transport
IN
    Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan
PA
    Board of Regents, The University of Texas System, USA
SO
    U.S. Pat. Appl. Publ., 41 pp., Cont.-in-part of U.S. Ser. No. 244,791.
    CODEN: USXXCO
DТ
    Patent
LA
    English
    ICM A01N025-00
IC
INCL 504116100
CC
    5-4 (Agrochemical Bioregulators)
FAN.CNT 3
    PATENT NO.
                      KIND
                             DATE
                                       APPLICATION NO.
                                                             DATE
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PΤ
    US 2002160915
                      A1
                             20021031
                                       US 2001-793336
                                                             20010226 <--
    US 6448472
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    US 2000-185299P
PRAI US 1999-244791
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CLASS
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PATENT NO.
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US 2002160915
               ICM
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US 2002160915
               NCL
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               ECLA
                      A01N037/28; A01N037/30; A01N061/00; C07K014/415;
                      C12N009/14; C12N015/82C4B; C12N015/82C8B4;
                      C12N015/82C8B; C12Q001/42
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US 6448472
                      435/468.000; 800/298.000; 800/300.000
               ECLA
                      C07K014/415; C12N009/14; C12N015/82C8B4
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The present invention relates to the modulation of pesticidal and

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RN

herbicidal activity by treatment of a membrane transport system in a cell. This entails modifying the extra-cellular phosphatases found in the membranes of these cells. By modifying the ATP gradient across the biol. membrane of a target plant, bacteria, insect or mammalian cell via inhibiting one or more extra-cellular phosphatases, it is possible to alter the sensitivity to a pesticide or herbicide. The method also comprises inhibiting an ABC transporter in the target cell. The method can also be used for identifying chems. with pesticidal activity. pesticidal herbicidal activity modulation animal plant plasma membrane transport; pesticide herbicide ectophosphatase ABC transporter inhibition Transport proteins RL: BSU (Biological study, unclassified); BIOL (Biological study) (ABC (ATP-binding cassette) transporters; enhancement of pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes and inhibiting an ABC transporter) Herbicides Pesticides (ectophosphatase inhibitors which enhance pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes) Pesticides (toxicity; ectophosphatase inhibitors which enhance pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes) 41481-51-0 139963-64-7 154201-55-5 168832-50-6 171248-07-0 291536-79-3 291536-80-6 291536-81-7 291536-82-8 291536-83-9 **291536-84-0** 291536-86-2 **291536-87-3** 291536-89-5 291536-90-8 291536-91-9 291536-92-0 291536-88-4 358622-53-4 RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses) (ectophosphatase inhibitor which enhances pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes) 56-65-5, ATP, biological studies RL: BSU (Biological study, unclassified); BIOL (Biological study) (ectophosphatase inhibitors which enhance pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes) 9032-64-8, Nucleotide pyrophosphatase 37289-25-1 ATP pyrophosphatase RL: BSU (Biological study, unclassified); BIOL (Biological study) (extracellular; ectophosphatase inhibitors which enhance pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes) 291536-82-8 291536-84-0 291536-87-3 358622-53-4 RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses) (ectophosphatase inhibitor which enhances pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes) 291536-82-8 HCAPLUS 1-Naphthaleneacetic acid, [(2-hydroxy-5-methylphenyl)methylene]hydrazide (CA INDEX NAME)

RN 291536-84-0 HCAPLUS
CN 1-Naphthaleneacetic acid, [(4-bromophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 291536-87-3 HCAPLUS
CN Acetic acid, (2,4,6-trimethylphenoxy)-, (phenylmethylene)hydrazide (9CI)
(CA INDEX NAME)

RN 358622-53-4 HCAPLUS

WO 2002020726

A3

20020606

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

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GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
            PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
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         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
            BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2001090710
                         A5
                               20020322
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     US 2002077365
                         A1
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PRAI US 2000-231088P
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CLASS
PATENT NO.
                CLASS
                       PATENT FAMILY CLASSIFICATION CODES
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WO 2002020726
                ICM
US 2002077365
                NCL
                       514/621.000; 504/329.000; 514/553.000; 504/149.000
                ECLA
                       A01N037/10; A01N037/22; A01N037/28; A01N037/28+M;
                       A01N037/30; A01N037/38; A01N037/46; A01N041/06;
                       A01N043/12; A01N043/16; A01N043/38; A01N043/78;
                       A01N047/06; A01N047/30; A01N047/44; A61K031/185;
                       C12N009/14; C12N015/82C8; C12N015/82C8B4
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GI

The present invention relates to methods for decreasing the resistance of AB microbial strains to antiinfectives such an antibiotics and antifungals by altering the ATP gradient across biol. membranes. The altering of the ATP gradient across biol. membranes is achieved through the inhibition of ecto-phosphatase activity and/or ABC transporter mol. activity which may be useful to reduce resistance in bacteria and yeast to aid in the treatment of certain infections and disease and to lower the concentration of antiinfectives necessary to inhibit the growth of microbial strains. Apyrase inhibitor I increased the growth inhibitory effect of the fungicide chlorothalonil by over 50%. Surflan was an equally effective weed killer against Arabidopsis thaliana at a five-fold less concentration in the presence of II. ST antiinfective enhancement inhibition ectophosphatase ABC transporter; ATP gradient biol membrane antibiotic antifungal

II

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transporter activities)

Drug screening

effectiveness; yeast bacteria resistance ectophosphatase ABC transporter; chlorothalonil fungicide enhancement apyrase inhibitor; surflan herbicide adjuvant apyrase inhibitor Transport proteins RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); BIOL (Biological study) (ABC (ATP-binding cassette) transporters; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) Gene, plant RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation) (AtPGP-1; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) Combinatorial library (DIVERSet format F, high throughput screening for apyrase inhibitors; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) P-glycoproteins RL: ADV (Adverse effect, including toxicity); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation) (MDR1; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) Agrochemical formulations (adjuvants; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) Fungicides (agrochem.; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) Membrane, biological (altering ATP gradient across; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) Plant cell (as target cell; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) Infection (bacterial; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) High throughput screening (drug, for apyrase inhibitors; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) Biological transport (efflux; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) Gene, plant RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation) (for apyrase; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC

(high throughput, for apyrase inhibitors; method for increasing effectiveness of antiinfective agents by inhibiting ectophosphatase and/or ABC transporter activities) IT Anti-infective agents (medical; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) TΤ Acaricides Algicides Animal Anti-infective agents Antibacterial agents Antibiotic resistance Antibiotics Antimicrobial agents Arabidopsis thaliana Bactericide resistance Drug delivery systems Drug resistance Embryophyta Eubacteria Fungicide resistance Fungicides Herbicide resistance Herbicides Human Insecticides Mammalia Multidrug resistance Nematocides Pesticides Pisum sativum Saccharomyces cerevisiae Yeast (method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) TT Multidrug resistance proteins RL: ADV (Adverse effect, including toxicity); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation) (method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) TΨ Pesticides (toxicity; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) TΤ Infection (yeast; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) IT 56-65-5, 5'-ATP, biological studies RL: BSU (Biological study, unclassified); CUS (Combinatorial use); BIOL (Biological study); CMBI (Combinatorial study); USES (Uses) (altering gradient of, across biol. membrane; method for increasing effectiveness of antiinfective agents by inhibiting ectophosphatase and/or ABC transporter activities) IT 41481-51-0 139963-64-7 154201-55-5 168832-50-6 171248-07-0 291536-79-3 291536-81-7 291536-82-8 291536-84-0 291536-86-2 **291536-87-3** 291536-88-4 291536-89-5 291536-90-8 291536-91-9 313493-42-4 403806-37-1

RL: BSU (Biological study, unclassified); CST (Combinatorial

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study, unclassified); BIOL (Biological study); CMBI
     (Combinatorial study)
        (as apyrase inhibitor; method for increasing effectiveness of
        antiinfective agents by inhibiting ecto-phosphatase and/or
        ABC transporter activities)
TT
     9000-95-7, Apyrase
     RL: ADV (Adverse effect, including toxicity); BSU (Biological study,
     unclassified); CUS (Combinatorial use); BIOL (Biological study); CMBI
     (Combinatorial study); USES (Uses)
        (ecto-; method for increasing effectiveness of antiinfective agents by
        inhibiting ecto-phosphatase and/or ABC transporter
        activities)
IT
     9000-83-3, ATPase
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (inhibition of, of ectophosphatase; method for increasing
        effectiveness of antiinfective agents by inhibiting ecto-
        phosphatase and/or ABC transporter activities)
IT
     19044-88-3, Surflan
                          40487-42-1, Pendimethalin
     RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL
     (Biological study); USES (Uses)
        (method for increasing effectiveness of antiinfective agents by
        inhibiting ecto-phosphatase and/or ABC transporter
        activities)
IT
     291536-80-6 291536-85-1
     RL: AGR (Agricultural use); DMA (Drug mechanism of
     action); BIOL (Biological study); USES (Uses)
        (method for increasing effectiveness of antiinfective agents by
        inhibiting ecto-phosphatase and/or ABC transporter
        activities)
IT
     145-63-1, Suramin
     RL: AGR (Agricultural use); DMA (Drug mechanism of action); PAC
     (Pharmacological activity); THU (Therapeutic use); BIOL (Biological
     study); USES (Uses)
        (method for increasing effectiveness of antiinfective agents by
        inhibiting ecto-phosphatase and/or ABC transporter
        activities)
IT
     66-81-9, Cycloheximide
                              2365-40-4, N6-(2-Isopentenyl) adenine
                                                                      3768-14-7,
     \alpha, \beta-Methyleneadenosine 5'-diphosphate
                                            28380-24-7, Nigericin
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (method for increasing effectiveness of antiinfective agents by
        inhibiting ecto-phosphatase and/or ABC transporter
        activities)
IT
     1897-45-6, Chlorothalonil
     RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
     THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (method for increasing effectiveness of antiinfective agents by
        inhibiting ecto-phosphatase and/or ABC transporter
        activities)
     291536-82-8 291536-84-0 291536-87-3
     RL: BSU (Biological study, unclassified); CST (Combinatorial
     study, unclassified); BIOL (Biological study); CMBI
     (Combinatorial study)
        (as apyrase inhibitor; method for increasing effectiveness of
        antiinfective agents by inhibiting ecto-phosphatase and/or
        ABC transporter activities)
RN
     291536-82-8 HCAPLUS
CN
     1-Naphthaleneacetic acid, [(2-hydroxy-5-methylphenyl)methylene]hydrazide
           (CA INDEX NAME)
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RN 291536-84-0 HCAPLUS

CN 1-Naphthaleneacetic acid, [(4-bromophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 291536-87-3 HCAPLUS

CN Acetic acid, (2,4,6-trimethylphenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

IT 9000-83-3, ATPase

RL: BSU (Biological study, unclassified); BIOL (Biological study) (inhibition of, of ectophosphatase; method for increasing effectiveness of antiinfective agents by inhibiting ectophosphatase and/or ABC transporter activities)

RN 9000-83-3 HCAPLUS

CN Phosphatase, adenosine tri- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

291536-85-1

RL: AGR (Agricultural use); DMA (Drug mechanism of action); BIOL (Biological study); USES (Uses) (method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities)

RN 291536-85-1 HCAPLUS

Benzoic acid, 3-methyl-, [1-(2-naphthalenyl)ethylidene]hydrazide (9CI) CN (CA INDEX NAME)

L146 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN AN2001:676991 HCAPLUS

DN 135:222868

ED Entered STN: 14 Sep 2001

TI Pesticide adjuvant activity through modulation of animal and plant cell membrane transport

IN Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan

PA Board of Regents of the University of Texas System, USA

SO PCT Int. Appl., 76 pp. CODEN: PIXXD2

DT Patent

LA English

IC ICM C12Q001-42

ICS C12Q001-34; C12Q001-00

CC 5-4 (Agrochemical Bioregulators)

FAN.CNT 1																			
	PATENT NO.					KIND		DATE		APPLICATION NO.						DATE			
PI	WO	WO 2001066792				A1 2001093			0913	WO 2001-US7423						20010307			
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			ZA,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM					•	
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			DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	
			ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG			
	US 2002103082					A1	A1 20020801				US 2001-800327						20010306		
	CA 2373424				AA	AA 20010913				CA 2001-2373424						20010307			
PRAI	US 2000-187819P				P 20000308														
	US 2001-800327				Α	A 20010306													
	WO	2001	-US74	423		W		2001	0307										
CLASS																			

CLASS PATENT FAMILY CLASSIFICATION CODES PATENT NO.

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______
                                             WO 2001066792
                ICM
                       C12Q001-42
                       C12Q001-34; C12Q001-00
                ICS
US 2002103082
                NCL
                       504/116.100; 504/117.000
                ECLA
                       C12Q001/42
AB
     The invention relates to the modulation of pesticidal and
    herbicidal activity by treatment of a membrane transport system in
     a cell. This entails modifying the extracellular phosphatases
     found in the membranes of these cells. By modifying the ATP gradient
     across the biol. membrane of a target plant, bacteria,
    insect or mammalian cell via inhibiting one or more extracellular
    phosphatases, it is possible to alter the sensitivity to a
    pesticide or herbicide. In preferred embodiments, the chemical
    moieties of the invention act as adjuvants to enhance pesticidal activity.
    pesticide adjuvant membrane extracellular phosphatase inhibition
ST
IT
     Transport proteins
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (ABC (ATP-binding cassette-
        containing); pesticide adjuvants acting by inhibition of
        extracellular phosphatases and ABC
        transporters)
IT
     Fungicides
        (fungicide adjuvants acting by inhibition of extracellular
       phosphatases in membranes)
IT
    Herbicides
        (herbicide adjuvants acting by inhibition of extracellular
       phosphatases in membranes)
IT
     Pesticides
        (pesticide adjuvants acting by inhibition of extracellular
        phosphatases in membranes)
IT
     9013-05-2, Phosphatase
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (ecto-; pesticide adjuvants acting by inhibition of extracellular
        phosphatases in membranes)
TT
     1897-45-6, Chlorothalonil
    RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
        (fungicide adjuvants acting by inhibition of extracellular
        phosphatases in membranes)
IT
     19044-88-3, Surflan
                          40487-42-1, Pendimethalin
     RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
        (herbicide adjuvants acting by inhibition of extracellular
        phosphatases in membranes)
IT
     41481-51-0
                 139963-64-7
                                154201-55-5
                                             168832-50-6
                                                            171248-07-0
                                291536-81-7 291536-82-8
     291536-79-3
                  291536-80-6
     291536-84-0 291536-85-1
                             291536-86-2 291536-87-3**
           291536-88-4
                        291536-89-5
                                      291536-90-8
                                                     291536-91-9
                                                                   291536-92-0
     313493-42-4
           ***AGR (Agricultural use); BIOL (Biological study);
     RL:
     USES (Uses)
        (pesticide adjuvant acting by inhibition of extracellular
        phosphatases in membranes)
     56-65-5, ATP, biological studies
IT
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (pesticide adjuvants acting by modification of ATP gradients across
        membranes)
RE.CNT
              THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Boyum; Biochem Biophys Res Commun 1997, V230, P22 HCAPLUS
(2) Decottignies; J Biol Chem 1998, V273(20), P12612 HCAPLUS
(3) Grant; Cancer Research 1994, V54, P357 HCAPLUS
```

```
(4) Thomas; The Plant Cell 2000, V12, P519 HCAPLUS
(5) University Of Texas; WO 0052144 Al 2000 HCAPLUS
     9013-05-2, Phosphatase
IT
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (ecto-; pesticide adjuvants acting by inhibition of extracellular
        phosphatases in membranes)
     9013-05-2 HCAPLUS
RN
                       (CA INDEX NAME)
CN
     Phosphatase (9CI)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     291536-82-8 291536-84-0 291536-85-1
     291536-87-3
     RL: AGR (Agricultural use); BIOL (Biological study);
     USES (Uses)
        (pesticide adjuvant acting by inhibition of extracellular
        phosphatases in membranes)
RN
     291536-82-8 HCAPLUS
     1-Naphthaleneacetic acid, [(2-hydroxy-5-methylphenyl)methylene]hydrazide
CN
     (9CI) (CA INDEX NAME)
```

RN 291536-84-0 HCAPLUS
CN 1-Naphthaleneacetic acid, [(4-bromophenyl)methylene]hydrazide (9CI) (CFINDEX NAME)

RN 291536-85-1 HCAPLUS

CN Benzoic acid, 3-methyl-, [1-(2-naphthalenyl)ethylidene]hydrazide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & O \\ \hline C & N-NH-C \\ \hline \end{array}$$

RN 291536-87-3 HCAPLUS

CN Acetic acid, (2,4,6-trimethylphenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L146 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:661570 HCAPLUS

DN 135:206922

ED Entered STN: 10 Sep 2001

TI Pesticidal and herbicidal activity through modulation of animal and plant cell membrane transport

IN Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan

PA Board of Regents, the University of Texas System, USA

SO PCT Int. Appl., 74 pp. CODEN: PIXXD2

DT Patent

LA English

IC C12N009-99; C12N015-01; A01H001-06

```
5-4 (Agrochemical Bioregulators)
FAN.CNT 3
   PATENT NO.
                       KIND
                              DATE
                                        APPLICATION NO.
                                                               DATE
                      _ - - -
                       A1 20010907 WO 2001-US6503
                                                               ------
    -----
                                                              20010227
    WO 2001064859
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
            HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
            LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
            SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU,
            ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ; TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
            BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI US 2000-185299P
                        P
                              20000228
CLASS
              CLASS PATENT FAMILY CLASSIFICATION CODES
PATENT NO.
 WO 2001064859 IC C12N009-99IC C12N015-01IC
                                                    A01H001-06
    The invention relates to the modulation of pesticidal and
    herbicidal activity by treatment of a membrane transport system in
    a cell. This entails modifying the extra-cellular phosphatases
    found in the membranes of these cells. By modifying the ATP gradient
    across the biol. membrane of a target plant, bacteria,
    insect or mammalian cell via inhibiting one or more extracellular
    phosphatases, it is possible to alter the sensitivity to a
    pesticide or herbicide. The method also comprises inhibiting an
    ABC transporter in the target cell. The method can also be used
    for identifying chems. with pesticidal activity.
ST
    pesticide herbicide ectophosphatase ABC
    transporter inhibition
    Transport proteins
IT
    RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
    (Biological study); PROC (Process)
       (ABC (ATP-binding cassette-
       containing); enhancement of pesticidal and herbicidal
       activity by altering the ATP gradient across biol. membranes and
       inhibiting an ABC transporter)
IT
    Herbicides
    Pesticides
       (ectophosphatase inhibitors which enhance pesticidal and
       herbicidal activity by altering the ATP gradient across biol.
       membranes)
    41481-51-0 139963-64-7 154201-55-5
TТ
                                          168832-50-6 171248-07-0
    291536-79-3 291536-80-6 291536-81-7 291536-82-8
    291536-83-9 291536-84-0 291536-86-2 291536-87-3
    291536-88-4 291536-89-5 291536-90-8 291536-91-9 291536-92-0
    358622-53-4
    RL: AGR (Agricultural use); BUU (Biological use,
    unclassified); BIOL (Biological study); USES (Uses)
       (ectophosphatase inhibitor which enhances pesticidal and
       herbicidal activity by altering the ATP gradient across biol.
       membranes)
IT
    56-65-5, ATP, biological studies
    RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
    (Biological study); PROC (Process)
       (ectophosphatase inhibitors which enhance pesticidal and
       herbicidal activity by altering the ATP gradient across biol.
       membranes)
IT
    9032-64-8, Nucleotide pyrophosphatase 37289-25-1
    , ATP pyrophosphatase
    RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
```

(Biological study); PROC (Process)

(extracellular; ectophosphatase inhibitors which enhance pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Lu, Y; The Plant Cell 1998, V10, P267 HCAPLUS
- (2) Thomas, C; The Plant Cell 2000, V12, P519 HCAPLUS

IT 291536-82-8 291536-84-0 291536-87-3

358622-53-4

RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses) (ectophosphatase inhibitor which enhances pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes)

RN 291536-82-8 HCAPLUS

CN 1-Naphthaleneacetic acid, [(2-hydroxy-5-methylphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 291536-84-0 HCAPLUS

CN 1-Naphthaleneacetic acid, [(4-bromophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 291536-87-3 HCAPLUS
CN Acetic acid, (2,4,6-trimethylphenoxy)-, (phenylmethylene)hydrazide (9CI)
(CA INDEX NAME)

IT 9032-64-8, Nucleotide pyrophosphatase 37289-25-1
, ATP pyrophosphatase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL

```
(Biological study); PROC (Process)
        (extracellular; ectophosphatase inhibitors which enhance
       pesticidal and herbicidal activity by altering the ATP
       gradient across biol. membranes)
RN
     9032-64-8 HCAPLUS
CN
     Pyrophosphatase, nucleotide (9CI)
                                       (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
    37289-25-1 HCAPLUS
CN
     Pyrophosphatase, adenosine triphosphate (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
L146 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
    2000:628251 HCAPLUS
DN
     133:219782
ED
    Entered STN: 10 Sep 2000
ΤI
    Genetic and epigenetic manipulation of ABC transporters and
     ecto-phosphatases for modulating drug resistance and methods for
     detection of ecto-phosphatase inhibitors
IN
     Thomas, Collin E.; Windsor, J. Brian; Roux, Stan
     J.; Lloyd, Alan M.; Hurley, Laurence
PA
    University of Texas, USA
SO
     PCT Int. Appl., 85 pp.
     CODEN: PIXXD2
DТ
    Patent
LA
    English
IC
     ICM C12N005-04
         C12N005-06; C12N001-16; C12N001-20; C12N015-67; C12N015-81;
         C12N015-82; C12N015-90; A01H001-00; A01H005-00
CC
     9-2 (Biochemical Methods)
     Section cross-reference(s): 1, 3, 10,
    11
FAN.CNT 3
    PATENT NO.
                        KIND
                                          APPLICATION NO.
                               DATE
                                                                DATE
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                               -----
                                          -----
PΙ
    WO 2000052144
                        A1
                               20000908
                                        WO 2000-US5315
                                                                20000228 <--
            AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
            CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
            IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
            MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
            SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
            DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
            CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                               20020313 EP 2000-913685
    EP 1185623
                         A1
                                                                 20000228 <--
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO
     US 2002173031
                        A1
                               20021121
                                         US 2002-47251
                                                                 20020114 <--
PRAI US 1999-261825
                               19990303
                         Α
                                        <--
    WO 2000-US5315
                         W
                               20000228
CLASS
PATENT NO.
                CLASS PATENT FAMILY CLASSIFICATION CODES
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                _ _ _ _
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WO 2000052144
                ICM
                       C12N005-04
                       C12N005-06; C12N001-16; C12N001-20; C12N015-67;
                ICS
                       C12N015-81; C12N015-82; C12N015-90; A01H001-00;
                       A01H005-00
US 2002173031
                NCL
                       435/245.000; 435/195.000
                ECLA
                       A61K031/165+A; A61K031/166; A61K031/167; A61K031/18;
                       A61K031/215L10; A61K031/216; A61K031/24; A61K031/352;
                       A61K031/381; A61K031/404; A61K031/425F; C07K014/705;
```

C12N009/14; C12N015/82C8B4

AΒ The present invention relates to methods for modulating the resistance of cells to foreign compds., i.e. drugs, antibiotics, etc. by altering the ATP gradient across biol. membranes. Altering the ATP gradient across biol. membranes is achieved through the manipulation of ectophosphatase activity and ABC transporter mol. activity. The above method may be useful to confer herbicide resistance to plants, antibiotic resistance to bacteria, and drug resistance to yeast cells, or to reduce resistance in cells, bacteria, and yeast in order to facilitate chemotherapeutic treatments. The present invention is also directed to the methods for identifying ecto-phosphatase inhibitors and uses thereof. Thus, Arabidopsis thaliana has been shown to possess an ecto-apyrase and this ecto-apyrase and PGP-1 (an MDR-like protein) to have a role in MDR. Addnl., the extracellular ATP pool was shown to be critical for MDR in yeast. Screening of a combinatorial library of small mols. has resulted in identification of apyrase inhibitors.

ST drug resistance ectophosphatase ABC transporter ATP gradient

IT Transport proteins

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(ABC; genetic and epigenetic manipulation of ABC transporters and ecto-phosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors).

IT Membrane, biological

(ATP gradient across; genetic and epigenetic manipulation of ABC transporters and ecto-phosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors)

IT Chemotherapy

Herbicide resistance

(augmentation of; genetic and epigenetic manipulation of ABC transporters and ecto-phosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors)

IT Neoplasm

(decreasing drug resistance in; genetic and epigenetic manipulation of ABC transporters and ecto-phosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors)

IT Arabidopsis thaliana

Aspergillus fumigatus

Bacteria (Eubacteria)

Drug resistance

Lactococcus lactis

Pea

Plant cell

Saccharomyces cerevisiae

Yeast

(genetic and epigenetic manipulation of ABC transporters and ecto-phosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors)

IT Animal cell

(mammalian; genetic and epigenetic manipulation of ABC transporters and ecto-phosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors)

IT 50-81-7, Ascorbic acid, uses 11098-84-3, Ammonium molybdate RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (genetic and epigenetic manipulation of ABC transporters and ecto-phosphatases for modulating drug resistance and methods for detection of ecto-phosphatase inhibitors)

```
IT
     9013-05-2, Phosphatase
                              41481-51-0
                                           139963-64-7
     154201-55-5
                   168832-50-6
                                 171248-07-0
                                               291536-79-3
                                                             291536-80-6
     291536-81-7 291536-82-8
                               291536-83-9 291536-84-0
                   291536-86-2 291536-87-3
     291536-85-1
                                             291536-88-4
     291536-89-5
                   291536-90-8
                                 291536-91-9
                                               291536-92-0
     RL: BAC (Biological activity or effector, except adverse);
     BSU (Biological study, unclassified); BIOL (Biological
     study)
        (genetic and epigenetic manipulation of ABC transporters and
        ecto-phosphatases for modulating drug resistance and methods
        for detection of ecto-phosphatase inhibitors)
TT
     56-65-5, ATP, biological studies
     RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
    BIOL (Biological study); OCCU (Occurrence)
        (gradient of; genetic and epigenetic manipulation of ABC
        transporters and ecto-phosphatases for modulating drug
       resistance and methods for detection of ecto-phosphatase
        inhibitors)
RE.CNT
              THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Decottignies; J Biol Chem 1998, V273(20), P12612 HCAPLUS
(2) Dudler; J Biol Chem 1992, V267(9), P5882 HCAPLUS
(3) Grant; Cancer Research 1994, V54, P357 HCAPLUS
(4) Kiba; Plant Cell Physiol 1995, V36(5), P809 HCAPLUS
(5) Lu; The Plant Cell 1998, V10, P267 HCAPLUS
(6) Sidler; The Plant Cell 1998, V10(10), P1632
(7) Thomas; Plant Physiol 1999, V119, P543 HCAPLUS
(8) Wang; J Biol Chem 1996, V271(17), P9898 HCAPLUS
     9013-05-2, Phosphatase 291536-82-8
     291536-84-0 291536-85-1 291536-87-3
    RL: BAC (Biological activity or effector, except adverse);
    BSU (Biological study, unclassified); BIOL (Biological
     study)
        (genetic and epigenetic manipulation of ABC transporters and
        ecto-phosphatases for modulating drug resistance and methods
        for detection of ecto-phosphatase inhibitors)
RN
     9013-05-2 HCAPLUS
CN
    Phosphatase (9CI)
                        (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
    291536-82-8 HCAPLUS
     1-Naphthaleneacetic acid, [(2-hydroxy-5-methylphenyl)methylene]hydrazide
CN
     (9CI)
           (CA INDEX NAME)
```

RN 291536-84-0 HCAPLUS
CN 1-Naphthaleneacetic acid, [(4-bromophenyl)methylene]hydrazide (9CI) (CAINDEX NAME)

RN 291536-87-3 HCAPLUS
CN Acetic acid, (2,4,6-trimethylphenoxy)-, (phenylmethylene)hydrazide (9CI)

(CA INDEX NAME)

L146 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:495114 HCAPLUS

DN 125:247329

ED Entered STN: 20 Aug 1996

TI Synthesis and antifungal activity of some new 2-methoxy-4-(N-substituted arylidene) phenoxyacetic acid hydrazides and their N-benzylidene derivatives

AU Joshi, P. C.

CS Chem. Lab., Kumaun Univ. Campus, Almora, 263 601, India

SO Asian Journal of Chemistry (1996), 8(3), 455-458

CODEN: AJCHEW; ISSN: 0970-7077

PB Asian Journal of Chemistry

DT Journal

LA English

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 5

GI

$$R - N = CH - OCH_2CONHR^1$$

AB Title compds. I (R = H, Me, Cl, Br, iodo; R1 = NH2, R2CH:N; R2 = Ph, substituted Ph) were prepared starting from etherification of 3,4-MeO(OH)C6H3CH:NC6H4R with ClCH2CO2Et. I (R = Me, R1 = PhCH:N, 4-O2NC6H4CH:N) showed antifungal activity against Alternaria alternata, Aspergillus flavus, and Fusarium moniliforme.

ST arylidenephenoxyacetic acid hydrazide prepn fungicide

IT Fungicides and Fungistats

(synthesis and antifungal activity of arylidenephenoxyacetic acid hydrazide derivs.)

IT51264-92-7P 51264-93-8P 51264-94-9P 53304-13-5P 53304-14-6P 78721-40-1P 181761-07-9P 181761-08-0P 181761-10-4P 181761-11-5P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (synthesis and antifungal activity of arylidenephenoxyacetic acid hydrazide derivs.)

IT 181761-12-6P 181761-13-7P 181761-15-9P 181761-16-0P 181761-22-8P 181761-18-2P 181761-20-6P 181761-21-7P 181761-24-0P 181761-25-1P 181761-26-2P 181761-27-3P 181761-30-8P 181761-32-0P 181761-34-2P 181761-36-4P 181761-38-6P 181761-41-1P 181761-44-4P 181761-47-7P 181761-50-2P 181761-53-5P 181761-57-9P 181761-61-5P 181761-64-8P

RL: BAC (Biological activity or effector, except adverse);

BSU (Biological study, unclassified); SPN (Synthetic preparation);
BIOL (Biological study); PREP (Preparation)
 (synthesis and antifungal activity of arylidenephenoxyacetic acid hydrazide derivs.)

TT 90-02-8, 2-Hydroxybenzaldehyde, reactions 100-52-7, Benzaldehyde, reactions 104-87-0, 4-Methylbenzaldehyde 105-39-5, Ethyl chloroacetate 123-11-5, 4-Methoxybenzaldehyde, reactions 555-16-8, 4-Nitrobenzaldehyde, reactions 3382-70-5 3382-71-6 17696-53-6 53304-12-4 58285-74-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis and antifungal activity of arylidenephenoxyacetic acid
 hydrazide derivs.)

IT 181761-12-6P 181761-20-6P 181761-26-2P 181761-36-4P 181761-50-2P

RL: BAC (Biological activity or effector, except adverse);
BSU (Biological study, unclassified); SPN (Synthetic preparation);
BIOL (Biological study); PREP (Preparation)

(synthesis and antifungal activity of arylidenephenoxyacetic acid hydrazide derivs.)

RN 181761-12-6 HCAPLUS

CN Acetic acid, [2-methoxy-4-{(phenylimino)methyl]phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

$$Ph-CH=N-NH-C-CH_2-O$$
OMe

RN 181761-20-6 HCAPLUS

CN Acetic acid, [2-methoxy-4-[[(4-methylphenyl)imino]methyl]phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{MeO} \\ & \text{O} \\ & \text{Ph-CH-N-NH-C-CH}_2-\text{O} \\ \end{array}$$

RN 181761-26-2 HCAPLUS

CN Acetic acid, [4-[[(4-chlorophenyl)imino]methyl]-2-methoxyphenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{MeO} & \text{CH} & \text{N} \\ & \text{O} & \\ & \text{Ph-CH} & \text{N-NH-C-CH}_2 - \text{O} \end{array}$$

RN 181761-36-4 HCAPLUS

CN Acetic acid, [4-[[(4-bromophenyl)imino]methyl]-2-methoxyphenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

RN 181761-50-2 HCAPLUS

CN Acetic acid, [4-[[(4-iodophenyl)imino]methyl]-2-methoxyphenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L146 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:610952 HCAPLUS

DN 109:210952

ED Entered STN: 10 Dec 1988

TI Synthesis of newer 5-chloro-2-phenylbenzimidazoles as potential antiviral agents. Part-LIII

AU Singh, Vijay LA.; Varma, Rajendra S.

CS Chem. Dep., Lucknow Univ., Lucknow, 226 007, India

SO Journal of the Indian Chemical Society (1988), 65(2), 139-40 CODEN: JICSAH; ISSN: 0019-4522

DT Journal

LA English

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 5

OS CASREACT 109:210952

GI

AB An acetohydrazide derivative underwent a condensation reaction with isatins to give hydrazones I (R1 = H, Me; R2 = H, Cl, Me, Br). Similarly prepared were benzaldehyde hydrazones II (R3 = H, OH; R4 = H, OMe). I and II exhibited plant antiviral activity.

I

ST benzimidazole carbamoylmethoxyphenyl prepn plant virucide;

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carbamylmethoxyphenylbenzimidazole prepn plant virucide;
    benzimidazolylphenoxyacetohydrazide prepn plant virucide
IT
    Virucides and Virustats
        (agrochem., [(carbamoylmethoxy)phenyl]benzimidazoles)
     302-01-2, Hydrazine, reactions
IT
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (amidation by, of (benzimidazolylphenoxy) acetate ester derivative)
                            90-02-8, Salicylaldehyde, reactions
IT
     87-48-9, 5-Bromoisatin
     Isatin 100-52-7, Benzaldehyde, reactions
                                                 123-11-5,
     4-Methoxybenzaldehyde, reactions
                                      608-05-9, 5-Methylisatin
                                                                   2058-74-4,
     1-Methylisatin 17630-76-1, 5-Chloroisatin
                                                  60434-13-1
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation reaction of, with (benzimidazolylphenoxy)acetohydrazide
       derivative)
IT
     95-83-0, 4-Chloro-1,2-benzenediamine
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation reaction of, with hydroxybenzoic acid)
IT
     99-96-7, 4-Hydroxybenzoic acid, reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation reaction of, with phenylenediamine derivative)
IT
     105-39-5, Ethyl chloroacetate
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (etherification by, of (hydroxyphenyl) benzimidazole derivative)
IT
     117332-23-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and amidation of, by hydrazine)
IT
     117332-24-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and condensation reaction of, with isatins and benzaldehydes)
IT
     113561-60-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and etherification of, by chloroacetate ester)
IT
     117332-25-9P
                   117332-26-0P 117332-27-1P
                                                 117332-28-2P
                                                                 117332-29-3P
     117332-30-6P 117332-31-7P
                               117332-32-8P
                                               117332-33-9P
    RL: BAC (Biological activity or effector, except adverse);
    BSU (Biological study, unclassified); SPN (Synthetic preparation);
    BIOL (Biological study); PREP (Preparation)
        (preparation and plant antiviral activity of)
IT
     117332-31-7P
    RL: BAC (Biological activity or effector, except adverse);
    BSU (Biological study, unclassified); SPN (Synthetic preparation);
    BIOL (Biological study); PREP (Preparation)
        (preparation and plant antiviral activity of)
     117332-31-7 HCAPLUS
RN
    Acetic acid, [4-(5-chloro-1H-benzimidazol-2-yl)phenoxy]-,
CN
     (phenylmethylene) hydrazide (9CI) (CA INDEX NAME)
```

L146 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1981:139699 HCAPLUS DN 94:139699

ED Entered STN: 12 May 1984

```
TI Synthesis and biological activity of some hydrazones and ureido oxadiazoles of 4-acetamidophenoxyacetic acid hydrazide
```

AU Shukla, M. K.; Singh, S. P.; Agarwal, V. K.

CS Dep. Chem., Lucknow Univ., Lucknow, 226 007, India

SO Current Science (1980), 49(24), 936-8 CODEN: CUSCAM; ISSN: 0011-3891

DT Journal

LA English

CC 28-11 (Heterocyclic Compounds (More Than One Hetero Atom)) Section cross-reference(s): 1, 5, 25

GI

ACNH
$$\longrightarrow$$
 OCH₂ \longrightarrow SCH₂CONHCONH \longrightarrow R

4-AcnHC6H4OCH2CONHN:CHC6H4R (I, R = H, 4-Me, 2-NO2, 3-NO2, 4-NO2, 2-OH, 4-OH, 2-Cl, 4-Cl, 2,4-Cl2, 4-NMe2, 4-NEt2) were obtained in 70-5% yield by treating 4-AcnHC6H4OCH2CONHNH2 (II) with RC6H4CHO. I are central nervous system depressants and I (R = 3-NO2, 4-Cl) had bactericidal activity against Bacillus subtilis. The oxadiazoles III (R = H, 2-Me, 4-Me, 2-OMe, 4-OMe) were obtained in 30-40% yield by treating II with CS2 and treating the resulting thiol with ClCH2CONHCONHC6H4R. III are virucidal and III (R = H, 2-Me, 4-OMe) have bactericidal activity.

ST benzaldehyde acetamidophenoxyacetylhydrazone; bactericide benzaldehyde acetamidophenoxyacetylhydrazone; central depressant benzaldehyde acetamidophenoxyacetylhydrazone; arylureidoacetylthiooxadiazole prepn virucide bactericide; oxadiazole arylureidoacetylthio

IT Virucides and Virustats

(acetamidophenoxymethyl (arylureidoacetylthio) oxadiazoles)

IT Central nervous system depressants

(benzaldehyde acetamidophenoxyacetylhydrazones)

IT Bactericides, Disinfectants and Antiseptics

(benzaldehyde acetamidophenoxyacetylhydrazones and acetamidophenoxymethyl(arylureidoacetylthio)oxadiazoles)

IT 77068-85-0P 77068-90-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and bactericidal and central nervous system depressant activity of)

IT 77068-82-7P 77068-83-8P 77068-84-9P 77068-86-1P

77068-87-2P 77068-88-3P 77068-89-4P 77068-91-8P 77068-92-9P

77068-93-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and central nervous system depressant activity of)

IT 77068-94-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with chloroacetylureas)

IT 77068-96-3P 77068-97-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and virucidal activity of)

IT 77068-95-2P 77068-98-5P 77074-20-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and virucidal and bactericidal activity of)

IT 75-15-0, reactions

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with acetamidophenoxyacetylhydrazine) 75129-75-8 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with aromatic aldehydes) 13558-76-4 13558-77-5 16615-79-5 IT 4791-23-5 13558-78-6 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with oxadiazolethiole)

IT 77068-82-7P

IT

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and central nervous system depressant activity of)

RN77068-82-7 HCAPLUS

Acetic acid, [4-(acetylamino)phenoxy]-, (phenylmethylene)hydrazide (9CI) CN (CA INDEX NAME)

L146 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

1976:442100 HCAPLUS AΝ

DN 85:42100

ED Entered STN: 12 May 1984

Phytotoxicity of hydrazones of aromatic aldehydes TI

AU Mazza, M.; Montanari, L.; Pavanetto, F.

Dep. Chim. Farm., Univ. Pavia, Pavia, Italy CS

SO Farmaco, Edizione Scientifica (1976), 31(5), 334-44 CODEN: FRPSAX; ISSN: 0430-0920

DT Journal

Italian LA

CC 5-3 (Agrochemicals)

Section cross-reference(s): 25

GI

$$X$$
 $CH = NR$
 I

AB The title compds. I (X and Y = H, OH, Me, OMe, halo, NO2, etc.; R = NHPh, NMePh, NMe2, NHAc and 1,2,4-triazolyl) and the related compds. were prepared and tested for herbicidal activity on 7 weed species. Most compds. were active, especially against Amaranthus retroflexus. The highest activity was shown i.e. by 4-(4-isopropylbenzylidene)amino-1,2,4triazole [32787-77-2], 2-methoxybenzaldehyde methylphenylhydrazone [23718-92-5] and salicylaldehyde methylphenylhydrazone [59670-28-9]. ST arom hydrazone herbicide

Herbicides IT

(aromatic aldehyde hydroazones)

IT Molecular structure-biological activity relationship (herbicidal, of aromatic aldehyde hydrazones)

IT 588-64-7P 610-64-0P 614-65-3P 622-73-1P 790-48-7P

```
1075-70-3P
             1216-15-5P
                           2216-75-3P
                                         2828-47-9P
                                                       2829-25-6P
2829-26-7P
             2829-27-8P
                           2829-28-9P
                                         2989-45-9P
                                                       3101-58-4P
                                         5051-49-0P
3681-18-3P
             5051-43-4P
                           5051-47-8P
                                                       5051-51-4P
5098-90-8P
             5941-05-9P
                           6579-24-4P
                                         7539-23-3P
                                                       10407-16-6P
10424-92-7P
              10424-94-9P
                             13405-65-7P
                                            13466-39-2P
                                                           14064-21-2P
14371-13-2P
                             14371-17-6P
                                            16435-03-3P
                                                           16435-04-4P
              14371-16-5P
16917-42-3P
              18998-48-6P
                             18998-49-7P
                                            18998-50-0P
                                                           18998-51-1P
                                            21968-29-6P
                                                           22699-29-2P
18998-53-3P
              21719-62-0P
                             21719-63-1P
              23550-76-7P
                                            23718-94-7P
22699-30-5P
                             23718-92-5P
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                                            24091-13-2P
23718-97-0P
              24090-98-0P
                             24090-99-1P
                                                           24091-14-3P
24459-52-7P
              24575-92-6P
                             25996-46-7P 25996-47-8P
25996-51-4P
              26090-73-3P
                             26090-77-7P
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32787-75-0P
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                                            32787-78-3P
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32787-80-7P
              32787-81-8P
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                                            32787-84-1P
                                                           33078-89-6P
34158-76-4P
              34948-39-5P
                             35546-29-3P
                                            35546-47-5P
                                                           35546-48-6P
35546-60-2P
              35546-62-4P
                             35546-65-7P
                                            35546-67-9P
                                                           35548-91-5P
35554-47-3P
              35554-48-4P
                             35558-91-9P
                                            35559-10-5P
                                                           42596-12-3P
42963-59-7P
              54009-61-9P
                             55754-32-0P
                                            56971-09-6P
                                                           58296-98-3P
59019-15-7P
              59473-50-6P
                             59670-10-9P
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59670-13-2P
              59670-14-3P
                             59670-15-4P
                                            59670-16-5P
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59670-18-7P
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59670-23-4P
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59670-28-9P
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                             59670-56-3P
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59670-59-6P
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                                                           59670-63-2P
59670-64-3P
              59670-65-4P
                             59670-66-5P
                                            59670-67-6P
                                                           59670-68-7P
59670-69-8P
              59670-70-1P
                             59670-71-2P
                                            59670-72-3P
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59670-74-5P
              59670-75-6P
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                                            59670-77-8P
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59670-79-0P
              59670-80-3P
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                                            59670-82-5P
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59670-84-7P
              59670-85-8P
                             59670-86-9P
                                            59670-87-0P
                                                           59670-88-1P
59670-89-2P
              59670-90-5P
                             59670-91-6P
                                            59694-69-8P
                                                           59694-70-1P
RL: AGR (Agricultural use); BAC (Biological activity or
effector, except adverse); BSU (Biological study,
unclassified); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation); USES (Uses)
   (preparation and herbicidal activity of)
25996-47-8P
RL: AGR (Agricultural use); BAC (Biological activity or
effector, except adverse); BSU (Biological study,
unclassified); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation); USES (Uses)
   (preparation and herbicidal activity of)
25996-47-8
           HCAPLUS
Acetic acid, [(4-nitrophenyl)methylene]hydrazide (9CI)
                                                           (CA INDEX NAME)
```

TT

RN

CN

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L146 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1974:82564 HCAPLUS
DN 80:82564
ED Entered STN: 12 May 1984
TI Enzyme inhibitors. IX. Preparation and in vitro study of
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```
N2-substituted hydrazides of 2-(5-methylindole)carboxylic and
     1-naphthylacetic acids as monoamineoxidase inhibitors
     Monge Vega, A.; Fernandez Alvarez, E.
ΑU
     Fac. Farm., Univ. Navarra, Pamplona, Spain
CS
     Anales de Quimica (1968-1979) (1973), 69(11), 1149-55
SO
     CODEN: ANOUBU; ISSN: 0365-4990
DT
     Journal
LA
     Spanish
     27-11 (Heterocyclic Compounds (One Hetero Atom))
CC
     Section cross-reference(s): 26
AB
     The hydrazides RCONHNHR1 (I, R = 5-methyl-2-indolyl, 1-naphthylmethyl, R1
     = C3-6 alkyl, phenylalkyl) were prepared by treating the hydrazides RCONHNH2
     with the aldehydes and reducing the hydrazones with NaBH4. I had 1-40
     times the monoamine oxidase-inhibiting activity of iproniazid.
ST
     hydrazide monoamine oxidase inhibitor; indolecarboxylic acid hydrazide;
     naphthylacetic acid hydrazide
IT
     609-14-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclization of, with p-toluidine)
IT
     9001-66-5
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (inhibitors of, indolecarboxylic and naphthylacetic acid hydrazides)
IT
     1463-64-5P
                  34800-90-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with aldehydes)
ΙT
     16382-15-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with hydrazine)
IT
     1086-51-7P
                  1086-52-8P 1094-37-7P
                                           51698-84-1P
                                                         51698-85-2P
     51698-86-3P
                   51698-87-4P
                                  51698-88-5P
                                                51698-89-6P
                                                               51698-90-9P
     51698-91-0P
                   51698-92-1P
                                  51698-93-2P
                                                51698-94-3P
                                                               51698-95-4P
     51698-96-5P
                   51698-97-6P
                                  51698-98-7P
                                                51698-99-8P
                                                               51699-00-4P
     51699-01-5P
                   51699-02-6P
                                  51699-03-7P
                                                51699-04-8P
                                                               51699-05-9P
     51699-06-0P
                   51699-07-1P
                                  51699-08-2P
                                                51699-09-3P
                                                               51699-10-6P
     51699-11-7P
                   51699-12-8P
                                  51699-13-9P
                                                51699-14-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
IT
     106-49-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with acetylacetate derivative)
IT
     1094-37-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     1094-37-7 HCAPLUS
CN
     1-Naphthaleneacetic acid, (phenylmethylene)hydrazide (9CI)
                                                                   (CA INDEX
     NAME)
```

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72:66627
DN
ED
    Entered STN: 12 May 1984
    Insecticidal arylhydrazones, hydrazines, and acylated amines
ΤI
PA
    Agripat S. A.
SO
    Fr., 13 pp.
    CODEN: FRXXAK
DT
    Patent
LA
    French
IC
    A01N
CC
    25 (Noncondensed Aromatic Compounds)
    PATENT NO.
                      KIND DATE APPLICATION NO.
                                                           DATE
    -----
                      ----
                             -----
                                        -----
    FR 1572191
                             19690627
                                                                       <--
PΙ
    CH 480790
                                        CH
    DE 1642214
                                        DE
                                         GB
    GB 1225357
    GB 1225358
                                         GB
    US 3549767
                             19700000
                                        US
                                                                       <--
PRAI CH
                             19661216 <--
CLASS
 PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
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              ____
 FR 1572191 IC
                      A01N
 US 3549767
              NCL
                      514/482.000; 514/464.000; 514/522.000; 514/599.000;
                      514/639.000
AB
    Hydrazones, hydrazines, and acylated amines with insecticidal
    properties are prepared Thus, iso-butylhydrazine 220 in 1:1 EtOH-H2O 400
    was added with stirring to 4'-chloroacetophenone 300 in EtOH 500 and AcOH
    20 parts, and the mixture heated to 70° to give N1-isobutyryl-N2-4'-
    chloroacetophenone hydrazone, m. 144-5° (EtOH-heptane). Also
    prepared was N1-(methoxythiocarbonyl)-N2-4'-chlorobenzaldehyde hydrazone, m.
    165-7° (MeOH) from methoxythiocarbonyl hydrazide and
    p-chlorobenzaldehyde. Sixty-four active compds. are prepared and
    insecticidal compns. are given.
ST
    insecticides hydrazones; hydrazones insecticides;
    hydrazines insecticides; acylamines insecticides
IT
    Hydrazones
    RL: RCT (Reactant); RACT (Reactant or reagent)
       (aryl, manufacture and insecticidal activity of)
IT
    Insecticides
       (hydrazones)
IT
    25415-88-7DP, Hydrazide, aryl
    RL: AGR (Agricultural use); BAC (Biological activity or effector, except
    adverse); BSU (Biological study, unclassified); SPN (Synthetic
    preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
       (preparation and insecticidal activity of)
IT
    3206-35-7P 3973-99-7P 5051-73-0P 6283-04-1P 6953-30-6P
    7151-53-3P 17655-31-1DP, Amide, N-(2-arylethyl), preparation
    25996-40-1P 25996-41-2P
                              25996-42-3P 25996-44-5P 25996-45-6P
    25996-46-7P 25996-47-8P 25996-48-9P
    25996-49-0P 25996-50-3P 25996-51-4P
                                          25996-52-5P
    25996-54-7P 25996-55-8P 25996-56-9P
                                          25996-57-0P 25996-58-1P
    25996-59-2P 25996-60-5P 25996-61-6P 25996-62-7P 25996-63-8P
    25996-64-9P 25996-65-0P 25996-66-1P 25996-67-2P 25996-68-3P
    25996-69-4P 25996-70-7P 25996-71-8P 25996-72-9P 25996-73-0P
    25996-74-1P 25996-76-3P 25996-77-4P 25996-78-5P 25996-79-6P
    25996-80-9P 25996-81-0P 25996-82-1P 25996-83-2P 25996-84-3P
                                           26011-68-7P 26011-69-8P
    25996-85-4P 25996-86-5P 25996-87-6P
    26011-71-2P 26011-72-3P 26011-73-4P
                                           26090-73-3P 26090-74-4P
    26090-75-5P 26090-77-7P 26090-78-8P
                                           26090-79-9P 26138-34-1P
    RL: SPN (Synthetic preparation); PREP (Preparation)
       (preparation of)
```

IT 25996-47-8P 25996-48-9P 25996-49-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 25996-47-8 HCAPLUS

CN Acetic acid, [(4-nitrophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 25996-48-9 HCAPLUS

CN Propionic acid, (p-nitrobenzylidene) hydrazide (8CI) (CA INDEX NAME)

RN 25996-49-0 HCAPLUS

CN Isobutyric acid, (p-nitrobenzylidene) hydrazide (8CI) (CA INDEX NAME)

L146 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1965:16315 HCAPLUS

DN 62:16315

OREF 62:2975a-e

ED Entered STN: 22 Apr 2001

TI Monoamine oxidase inhibitors. III. Hydrazine derivatives of certain arylacetic acids

AU Bojarska-Dahlig, Halina

CS Inst. Farm., Warsaw

SO Acta Polon. Pharm. (1963), 20(4), 293-302

DT Journal

LA Polish

CC 57 (Enzymes)

AB cf. CA 60, 9268c. Compds. of formula PhCH2CONHN:C(R)R1 (I) and 1-C10H7CH2CONHN:C(R)R1 (II) were prepared and tested in vitro for monoamine oxidase inhibition. To prepare the intermediate compds., PhCH2CONHNHCH(R)R1 (III) and 1-C10H7CH2CONHNHCH(R)R1 (IV), resp., 0.01 mole arylacetylhydrazine in 25 ml. 50% EtOH was treated with 0.01 mole carbonyl compound in a min. amount of 50% EtOH, the mixture refluxed 1 hr., most of the EtOH distilled, and the residue neutralized with NaHCO3. III (or IV) (0.05 mole) dissolved in 300 ml. EtOH, hydrogenated 3 hrs. at 70° and 40 atmospheric with 1.5 g. 10% Pd-carbon, the mixture filtered, the filtrate concentrated,

and the residue treated, if necessary, with petr. ether yielded I (or II). Given are R, R1, % yield of I, m.p. I, % yield of III, m.p. III, % inhibition of monoamine oxidase by III, that of PhCH2CH2NHNH2 in 10-4M concentration being considered 100%, and molarity of III solns. used in biol. testing: H, Ph, 84, 147-8° (EtOH), 79, 113.5-14°, 59, 10-4;

```
H, 2-pyridyl, 90, 163-3.5°, 70, 91-2° (EtOH), 83, 10-4; H,
3-pyridyl, 93, 144-5°, 90, 83.5-4° (AcOEt-petr. ether) 77,
10-4; H, 4-pyridyl, 96, 154-5°, 75, 94-5° (EtOH-petr.
ether), 84, 10-4; Me, Ph, 100, 158-60.5°, hydrogenation failed; Me,
2-pyridyl, 74, 144-5° (EtOH), 86, 118-19.5° (EtOH), 57,
10-4; Me, 3-pyridyl, 69, 136-8°, 53, 102-5° (HCl salt), 51,
10-4; Me, 4-pyridyl, 93, 148.5-9.5°, 52, 104.5-5°
(EtOH-petr. ether), 30, 10-4; Me, Me, 49, 197-8°, hydrogenation
failed; Me, Pr, 69, 111-11.5°, hydrogenation failed; Me,
3-carbazolyl, 65, 219-20° (EtOH), hydrogenation failed; analogous
data for II and IV are: H, Ph, 95, 215-15.5°, 77, 107-8°
(EtOH), 78, 10-4; H, 2-pyridyl, 65, 150-2.5°, 72, 156.5-7°,
48, 10-5; H, 3-pyridyl, 65, 194-6°, 77, 150.5° (AcOEt-petr.
ether) (the HCl salt m. 225° with decomposition), 75, 10-5 (the HCl
salt, 70 and 10-4); H, 4-pyridyl, 94, 176-8°, 84, 85-6°
(AcOEt), 74, 10-4; Me, Ph, 88, 135-8°, 80, 65-6°, 66, 10-4;
Me, 2-pyridyl, 91, 190-2°, 33, 99-9.5°, --, --; Me,
3-pyridyl, 94, 171-2°, hydrogenation failed; Me, 4-pyridyl, 99,
166-8°, 53, -- (the HCl salt m. 170-3° with decomposition), 68,
10-4 (biol. data refer to the HCl salt); Me, Me, 52, 104-5.5°
(EtOH), 40, 124-4.5°, 37, 10-4. The recrystn. solvent was dilute
EtOH unless otherwise stated. With I (R = H, R1 = 2-pyridyl), dilution of
the mother liquors left behind the 1st crop yielded an isomeric compound, m.
99.5-100.5° (EtOH). Refluxing 4 hrs. 12.5 g. o-
C6H4 (CH2CO2Et) 2 and 20 g. 40% (NH2) 2.H2O gave 9.5 g. o-
C6H4 (CH2CONHNH2) 2, m. 203-4.5°. o-C6H4 (CH2CONHN: CHPh) 2
(V), m. 236-7°, was prepared in 88% by the method used for preparation of
I and II. Hydrogenated 5 hrs. as above, V yielded 74%
o-C6H4 (CH2CONHNHCH2Ph)2, m. 150-50.5°, (EtOH); in biol.
tests, it gave 74% inhibition in 10-4M concentration An analogous hydrazone
also prepared from o-C6H4(CH2CONHNH2)2 and 2-pyridinecarboxaldehyde
in 88%; m.p. 238-9° (C5H5N); its hydrogenation failed.
1087-36-1, Acetic acid, phenyl-, benzylidenehydrazide
                                                        1245-39-2,
Acetic acid, phenyl-, (1-carbazol-3-ylethylidene)hydrazide
   (amino oxidase inhibition by)
9059-11-4, Amine oxidase
   (arylacetic acid hydrazine derivative effect on)
1088-99-9, Acetic acid, phenyl-, 2-[1-(3-pyridyl)ethyl]hydrazide,
dihydrochloride
   (prepn of, and amino oxidase inhibition by)
1080-09-7, Acetic acid, phenyl-, isopropylidenehydrazide
                                                            1083-03-0,
o-Benzenediacetic acid, dihydrazide
                                      1083-52-9, Acetic acid, phenyl-,
(1-methylbutylidene)hydrazide
                              1086-51-7, 1-Naphthaleneacetic acid,
2-isopropylhydrazide
                       1086-52-8, 1-Naphthaleneacetic acid,
isopropylidenehydrazide
                          1087-37-2, Acetic acid, phenyl-,
                               1087-38-3, Acetic acid, phenyl-,
2-(4-pyridylmethyl)hydrazide
                                1087-39-4, Acetic acid, phenyl-,
(4-pyridylmethylene)hydrazide
2-(3-pyridylmethyl)hydrazide
                               1087-40-7, Acetic acid, phenyl-,
(3-pyridylmethylene) hydrazide
                                1087-41-8, Acetic acid, phenyl-,
2-(2-pyridylmethyl)hydrazide
                               1087-42-9, Acetic acid, phenyl-,
                                1088-96-6, Acetic acid, phenyl-,
(2-pyridylmethylene) hydrazide
(α-methylbenzylidene) hydrazide
                                 1088-97-7, Acetic acid, phenyl-,
2-{1-(4-pyridyl)ethyl]hydrazide
                                  1088-98-8, Acetic acid, phenyl-,
[1-(4-pyridyl)ethylidene]hydrazide
                                     1089-00-5, Acetic acid, phenyl-,
                                     1089-01-6, Acetic acid, phenyl-,
[1-(3-pyridyl)ethylidene]hydrazide
2-[1-(2-pyridyl)ethyl]hydrazide
                                 ·1089-02-7, Acetic acid, phenyl-,
[1-(2-pyridyl)ethylidene]hydrazide
                                     1094-36-6, 1-Naphthaleneacetic acid,
2-benzylhydrazide 1094-37-7, 1-Naphthaleneacetic acid,
benzylidenehydrazide
                       1094-38-8, 1-Naphthaleneacetic acid,
2-(4-pyridylmethyl)hydrazide
                               1094-39-9, 1-Naphthaleneacetic acid,
(4-pyridylmethylene)hydrazide
                               1094-40-2, 1-Naphthaleneacetic acid,
2-(3-pyridylmethyl)hydrazide
                               1094-41-3, 1-Naphthaleneacetic acid,
```

was

IT

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IT

IT

2-(3-pyridylmethyl)hydrazide, dihydrochloride 1094-42-4, 1-Naphthaleneacetic acid, (3-pyridylmethylene)hydrazide 1094-43-5, 1-Naphthaleneacetic acid, 2-(2-pyridylmethyl)hydrazide 1094-44-6, 1-Naphthaleneacetic acid, (2-pyridylmethylene)hydrazide 1096-98-6, 1-Naphthaleneacetic acid, 2-(α-methylbenzyl)hydrazide 1096-99-7, 1-Naphthaleneacetic acid, (α-methylbenzylidene) hydrazide 1097-00-3, 1-Naphthaleneacetic acid, 2-[1-(4-pyridyl)ethyl]hydrazide, dihydrochloride 1097-01-4, 1-Naphthaleneacetic acid, [1-(4-pyridyl)ethylidene]hydrazide 1097-02-5, 1-Naphthaleneacetic acid, [1-(3-pyridyl)ethylidene]hydrazide 1097-03-6, 1-Naphthaleneacetic acid, 2-[1-(2-pyridyl)ethyl]hydrazide 1097-04-7, 1-Naphthaleneacetic acid, [1-(2-pyridyl)ethylidene]hydrazide 1106-90-7, o-Benzenediacetic acid, bis(2-benzylhydrazide) 1106-91-8, o-Benzenediacetic acid, bis(benzylidenehydrazide) 1106-92-9, o-Benzenediacetic acid, bis[(2-pyridylmethylene)hydrazide] (preparation of, and amino oxidase inhibition by) 1087-36-1, Acetic acid, phenyl-, benzylidenehydrazide IT (amino oxidase inhibition by) 1087-36-1 HCAPLUS RNBenzeneacetic acid, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME) CN

RN 1106-91-8 HCAPLUS
CN o-Benzenediacetic acid, bis(benzylidenehydrazide) (7CI, 8CI) (CA INDEX NAME)

L146 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1964:440228 HCAPLUS DN 61:40228

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OREF 61:6955d-f
ED
    Entered STN: 22 Apr 2001
    N-Halo-N-methyl-N'-phenylureas
ΤI
    Loux, Harvey M.
IN
PA
    E. I. du Pont de Nemours & Co.
SO
    5 pp.
DT
    Patent
    Unavailable
LA
INCL 260553000
    35 (Noncondensed Aromatic Compounds)
    PATENT NO. KIND DATE
                                         APPLICATION NO.
                                                               DATE
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                              -----
                                         ______
                                                               _____
    US 3141038
                              19640714
PΙ
                                                               19611113 <--
CLASS
PATENT NO.
              CLASS PATENT FAMILY CLASSIFICATION CODES
               ____
 -----
US 3141038
              INCL
                      260553000
US 3141038
              NCL
                      562/801.000; 504/330.000; 558/314.000
    For diagram(s), see printed CA Issue.
GI
AB
    The title compds. were prepared by direct halogenation of the appropriate
    corresponding methylurea. Thus, to a stirred solution of 0.25 mole
    3,4-Cl2C6H3NHCONHMe and 0.25 mole NaOAc in 1200 ml. HOAc, 0.25 mole Cl was
    added at 17° during 10 min. and the mixture stirred an addnl. 0.5 hr.
    to give I (R = R1 = H, R2 = R3 = R4 = C1), m. 229°, and a filtrate
    which yielded I (R = R3 = R4 = C1, R1 = R2 = H) (II). To 345 ml. 1.1N
    ethereal solution of MeNHCl, 70 ml. 1.06N hexane solution of 3,4- Cl2C6H3NCO
was
    added with stirring at 25° and the mixture stirred an addnl. 1 hr. to
    give 91.5% II, m. 96.5-7.5° (hexane). To a N hexane solution of
    3,4-Cl2C6H3NMeCOCl, an ethereal solution which was N both in MeNHCl and Me3N
    was added and the mixture stirred 2 hrs. to give I (R = R3 = R4 = Cl, R1 =
    Me, R2 = H). Many analogs of these compds. were reported with no phys.
    data. These compds. possess outstanding herbicidal activity.
TT
    1080-09-7, Acetic acid, phenyl-, isopropylidenehydrazide 1087-36-1
    , Acetic acid, phenyl-, benzylidenehydrazide 89938-88-5, Urea,
    1-chloro-3-(3,4-dichlorophenyl)-1-methyl- 89938-89-6, Urea,
    1-methyl-3-(2,3,4-trichlorophenyl) - 90003-44-4, Urea,
    1-chloro-3-(p-chlorophenyl)-1-methyl- 92032-34-3, Butyric acid,
    2-phenyl-, isopropylidenehydrazide
       (preparation of)
IT
    1087-36-1, Acetic acid, phenyl-, benzylidenehydrazide
       (preparation of)
RN
    1087-36-1 HCAPLUS
CN
    Benzeneacetic acid, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)
```

=> => d l148 bib abs hitstr retable tot

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L148 ANSWER 1 OF 45 HCAPLUS COPYRIGHT 2005 ACS on STN AN 2000:304195 HCAPLUS
DN 133:30462
TI Infrared spectra and electrical conductivity of som
```

TI Infrared spectra and electrical conductivity of some hydrazones

AU Shabana, Ahmed A.

Ph-CH=N-NH-C-CH2-Ph

CS Department of Chemistry, Faculty of Science, Al-Azhar University, Nasr City, Cairo, 11884, Egypt

SO Canadian Journal of Analytical Sciences and Spectroscopy (1999),

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L58 ANSWER 1 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:809047 HCAPLUS

DN 132:166181

TI Synthesis of some thiazolidinone and triazole derivatives of expected antimicrobial activity

AU Mohamed, Shadia R.

CS Pharmaceutical Chemistry Department, Faculty of Pharmacy, Cairo University, Cairo, Egypt

SO Bulletin of the Faculty of Pharmacy (Cairo University) (1999), 37(2), 33-40

Ι

CODEN: BFPHA8; ISSN: 1110-0931

PB Cairo University, Faculty of Pharmacy

DT Journal

LA English

GI

AB New derivs. of semicarbazide and thiosemicarbazide have been synthesized together with new substituted alkyl and aryl 1,2,4-triazoles and a thiazolidinone obtained by cyclizing the appropriate thiosemicarbazide. Screening for antibacterial and antifungal activities using preliminary

scan by the agar plate inhibition zone method, followed by MIC vs. ampicillin and clotrimazole, revealed high activity for compds. I and II. The partition coeffs. of the most and least biol. active compds. were determined

IT 259104-26-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 259104-26-2 HCAPLUS

CN. Acetic acid, [4-(acetylamino)-3-methylphenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
	+=====	+====: ·	+=====	+=====================================	+=======
Anon	1967	I	666	SPP Rev Captrider An	
Bhamaria, R	1968	6	61	J Exp Biol	
Budavari, S			1083	The Merck INDEX, 12t	
Carlson, H	1948	55	607	J Bacteriol	
Chandra, S	1968	31	117	Indian J Appl Chem	HCAPLUS
Epstein, J	1944	29	319	Lab Clin Med	HCAPLUS
Foye, W	1995		809	Principles of Medici	
Fukujiro, F	1968	88	1423	Yakugaku Zasshi	HCAPLUS
Gupta, A	1979	56	1230	J Indian Chem Soc	
Irving, G	1946	52	10	J Bacteriol	
Jack, D	1988	452	257	J Chromatogr	HCAPLUS
Pathak, R	1980	8	12	J Antibact Antifung	
Pitt, J	1979	57	2021	Can J Bot	
Samson, R	1976		1	Stud Mycol	
Seoh, L	1981	14	231	Chayon kwahak pyon (HCAPLUS
Singh, S	1981	81	175	Chem Rev	HCAPLUS
Stefan, J	1970		İ	DE 1953149 `	HCAPLUS
Stefan, J	1968	ĺ	İ	Swiss Appl	HCAPLUS

L58 ANSWER 2 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:775321 HCAPLUS

DN 130:110191

TI Synthesis and antitubercular activity of novel thiazolidinone derivatives

AU Oza, Haresh; Joshi, Dharti; Parekh, Hansa

CS Department of Chemistry, Saurashtra University, Rajkot, 360 005, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1998), 37B(8), 822-824 CODEN: IJSBDB; ISSN: 0376-4699

PB National Institute of Science Communication, CSIR

DT Journal

LA English

GI

$$\begin{array}{c|c} O & O & \\ \hline \\ Me & N & \\ \hline \\ H & \\ H & \\ \end{array}$$
 N=CHR II

AB Thirty thiazolidinones I (R = Ph, ClC6H4, 4-Me2NC6H4, HOC6H4, O2NC6H4, PhCH:CH, etc.; R1 = H, Me) were prepared by cyclocondensation of Schiff bases II with thioglycolic acid and thiolactic acid. All I were screened for antitubercular activity against Mycobacterium tuberculosis H37 Rv.

IT 77068-82-7P

Ι

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of antitubercular [(acetamidophenoxy)acetamido]thiazolidinones by cyclocondensation of [(acetamidophenoxy)acetyl hydrazide Schiff bases with thioglycolate or thiolactate)

RN 77068-82-7 HCAPLUS

CN Acetic acid, [4-(acetylamino)phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File		
Anon	1992	İ			HCAPLUS		
Anon	1993			·	HCAPLUS		
Anon	1994	İ			HCAPLUS		
Anon	1996	İ	Ì		HCAPLUS		
Anon	1996		Ì		HCAPLUS		
Bianchi, M	1996	117	130	Br J Pharmacol	HCAPLUS		
Bjune, K	1996	40	399	Acta Anaestheriol Sc	HCAPLUS		
Claris, D	1991	•		ZA 9201			
Hogale, M	1991	30B	717	Indian J Chem	HCAPLUS		
Ladva, K	1991	68	379	J Indian Chem Soc			
Nargund, L	1996	35B	499	Indian J Chem	HCAPLUS		
Pandya, D	1993	48	414	Pharemazie	HCAPLUS		
Vashi, B	1995	34B	802	Indian J Chem	HCAPLUS		
Viltaria, D	1992	35	2910	J Med Chem			

L58 ANSWER 3 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:529514 HCAPLUS

DN 127:205529

TI Studies on some 2-aryl-5-p-chlorophenoxymethylene-Δ2-1,3,4-

oxadiazolines

AU Tiperciuc, Brandusa; Ghiran, Doina; Verite, Philippe

CS Facultatea de Farmacie, U. M. F., Iuliu Hatieganu, Rom.

SO Clujul Medical (1997), 70(1), 85-90 CODEN: CLUMBY; ISSN: 0257-7267

PB Institutul de Medicina si Farmacie Cluj-Napoca

DT Journal

LA Romanian

GI

$$C1 - OCH_2 - OCH_2 - R$$

AB Title compds. I [R = H, 2-OAc, 3-OAc, 4-OAc, 2-OMe, 3-OMe, 4-OMe, 2-Cl, 3-Cl, 4-Cl] were prepared by treating 4-ClC6H4OCH2CONHNH2 with RC6H4CHo and cyclization with Ac2O. I have antimicrobial activity at 10 mg/mL.

IT 2503-75-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of bactericidal chlorophenoxymethyleneoxadiazolines)

RN 2503-75-5 HCAPLUS

L58 ANSWER 4 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:277905 HCAPLUS

DN 127:17543

TI 2-Azetidinone: 2-aryl-1-(2',4',6'-trichlorophenoxyacetamido)-3-chloro-2-azetidinone

AU Sorathiya, S. D.; Patel, V. B.; Parikh, A. R.

CS Chem. Dep., Saurashtra Univ., Rajkot, India

SO Journal of the Institution of Chemists (India) (1996), 68(6), 177-179

CODEN: JOICA7; ISSN: 0020-3254

PB Institution of Chemists (India)

DT Journal

LA English

GI

$$C1$$
 OCH_2CONH
 R
 $C1$
 O
 $C1$
 O
 $C1$
 O
 $C1$

AB A series of 2-azetidinone derivs., I (R = Ph, 4-ClC6H4, 2-HOC6H4, etc.), bearing 2, 4, 6-trichlorophenoxyacetic acid hydrazide moiety have been synthesized and their antimicrobial activity studied.

IT 190588-44-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, bactericidal, and fungicidal activity of (trichlorophenoxyacetamido) azetidinones)

RN 190588-44-4 HCAPLUS

CN Acetic acid, (2,4,6-trichlorophenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

RETABLE

Referenced Author (RAU)	•	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Kamaiya, T Maffi, G Roger, D	1977 1959 	1		Spec Phbl Chem Soc Ed Sci US 39558974	

L58 ANSWER 5 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:607951 HCAPLUS

DN 125:301247

TI Synthesis and biological screening of substituted thymolylthiazolidinones and thymolylazetidinones

AU Vashi, B. S.; Shah, V. H.

CS Dep. Chem., Saurashtra Univ., Rajkot, 360 005, India

SO Journal of the Indian Chemical Society (1996), 73(9), 491-492 CODEN: JICSAH; ISSN: 0019-4522

PB Indian Chemical Society

DT Journal

LA English

GI

ON
$$R^1$$
 OCH2CONH $CHMe_2$ N R^1 OCH_2CONH OCH

AB The present communication reports the synthesis of thymolyl derivs. of 4-thiazolidinones and azetidinones. The compds. have been tested for antibacterial and antifungal activity. P-Nitrosothymol (I; R = H) on condensation with Et chloroacetate, followed by the action of hydrazine hydrate yielded O-(hydrazinocarbonylmethyl)-p-nitrosothymol (I; R = CH2CONHNH2). The later on condensation with different aromatic aldehydes yielded the azomethine derivs. (I; R = CH2CONHN:CHR1, R1 = Ph, 3-, 4-H2NC6H4, 2-, 3-, 4-ClC6H4, 2,6-, 3,4-Cl2C6H3, 2-, 3-, 4-HOC6H4, 4-MeOC6H4, 2-, 3-, 4-O2NC6H4). Compds. I (R = CH2CONHN:CHR1) on cyclocondensation with thioglycolic and thiolactic acid yielded 4-thiazolidinones (II; R2 = H, Me, resp.) and with thiomalic acid in presence of anhydrous zinc chloride yielded 4-thiazolidinones (II; R2 = CH2CO2H). The four-membered β -lactam ring is introduced in I (R = CH2CONHN: CHR1) by cycloaddn. of chloroacetyl chloride in presence of triethylamine to yield 2-azetidinones III.

IT 182867-02-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (synthesis and bioactivity of substituted thymolylthiazolidinones and -azetidinones)

RN 182867-02-3 HCAPLUS

CN Acetic acid, [5-methyl-2-(1-methylethyl)-4-nitrosophenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

AN 1996:488265 HCAPLUS

DN 125:212091

TI Preparation and pharmacology of N-acylhydrazones

AU Dilanyan, E. R.; Arsenyan, F. G.; Stepanyan, G. M.; Akopyan, L. G.

CS Inst. Fine Organic Chem. Armenia, Yerevan, Armenia

SO Khimiko-Farmatsevticheskii Zhurnal (1996), 30(6), 16-17 CODEN: KHFZAN; ISSN: 0023-1134

PB Izdatel'stvo Folium

DT Journal

LA Russian

AB Treatment of aldehydes or ketones with 4-alkoxyphenylacetic acid hydrazides, gave the corresponding N-(4-alkoxyphenylacetyl)hydrazones. The hydrazones were tested for antitumor, antimicrobial, mutagenic, and anticonvulsant activities.

IT 181428-40-0P 181428-47-7P 181428-53-5P 181428-59-1P 181428-64-8P 181428-70-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and pharmacol. of N-acylhydrazones)

RN 181428-40-0 HCAPLUS

CN Benzeneacetic acid, 4-methoxy-, [(2-hydroxyphenyl)methylene]hydrazide (9CI). (CA INDEX NAME)

RN 181428-47-7 HCAPLUS

CN Benzeneacetic acid, 4-ethoxy-, [(2-hydroxyphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 181428-53-5 HCAPLUS

CN Benzeneacetic acid, 4-(1-methylethoxy)-, [(2-hydroxyphenyl)methylene]hydra zide (9CI) (CA INDEX NAME)

RN 181428-59-1 HCAPLUS

CN Benzeneacetic acid, 3-bromo-4-methoxy-, [(2-hydroxyphenyl)methylene]hydraz ide (9CI) (CA INDEX NAME)

RN 181428-64-8 HCAPLUS

CN Benzeneacetic acid, 3-bromo-4-ethoxy-, [(2-hydroxyphenyl)methylene]hydrazi de (9CI) (CA INDEX NAME)

RN 181428-70-6 HCAPLUS

CN Benzeneacetic acid, 3-bromo-4-(1-methylethoxy)-, [(2-hydroxyphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 7 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:149553 HCAPLUS

DN 124:289433

TI Synthesis and antimicrobial activity of certain arylidene derivatives of 6-iodo-2-phenyl-3-(4-hydrazinocarbonylmethoxyphenyl)-4(3H)-quinazolinones

AU Aziza, M. A.; Ibrahim, M. K.; El-Hamide, S. G. Abd; Hakim, A. E.

CS Faculty Pharmacy, Al-Azhar University, Cairo, Egypt

SO Al-Azhar Journal of Pharmaceutical Sciences (1994), 14, 202-9 CODEN: AAJPFT; ISSN: 1110-1644

PB Al-Azhar University, Faculty of Pharmacy

DT Journal

LA English

GI

AB The synthesis of 4(3H)-quinazolinones I (R = H, Me, Et; X = H, 4-Me, 4-MeO, 2-, 3-, 4-Cl, 4-HO) was carried out. The antimicrobial screening has shown that some of these compds. were active against microorganisms. None were active against E. coli.

IT 175851-66-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

Ι

(preparation and bactericidal activity of iodophenylquinazolinones)

RN 175851-66-8 HCAPLUS

CN Acetic acid, [4-(6-iodo-4-oxo-2-phenyl-3(4H)-quinazolinyl)phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 8 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:123209 HCAPLUS

DN 124:219420

TI Structural modification of the primary amino group of anticonvulsant aryl semicarbazones

AU Dimmock, J. R.; Puthucode, R. N.; Lo, M. S.; Quail, J. W.; Yang, J.; Stables, J. P.

CS Coll. Pharmacy and Nutrition, Univ. Saskatchewan, Saskatoon, SK, Can.

SO Pharmazie (1996), 51(2), 83-8 CODEN: PHARAT; ISSN: 0031-7144

PB Govi-Verlag Pharmazeutischer Verlag

DT Journal

LA English

AB A number of arylsemicarbazones were shown previously to have significant anticonvulsant properties. The importance of the primary amino group in a series of compds. was determined by replacing it with other substituents. The amino group was not essential for anticonvulsant activity. However, its replacement by an aryl ring generally abolished the activity, while a terminal phenylamino function was better tolerated. Thus both the size of the group and its H-bonding capabilities appear to influence the bioactivity. Alteration of the O atom of the semicarbazones by isosteres did not enhance anticonvulsant properties.

IT 130158-81-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)
(primary amino group modification of anticonvulsant arylsemicarbazones)
130158-81-5 HCAPLUS
Benzoic acid, 4-methyl-, (1-phenylethylidene)hydrazide (9CI) (CA INDEX

L58 ANSWER 9 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:116243 HCAPLUS

DN 124:260935

NAME)

RN

CN

TI Synthesis and antimicrobial activities of some new benzimidazoles, Part I

AU El-Sherief, H. A.; El-Ezbawy, S. R.; Mahmoud, A. M.; Sarhan, Abd El-Wareth A. O.

CS Faculty Science, Assiut University, Assiut, Egypt

SO Bulletin of the Faculty of Science, Assiut University, B: Chemistry (
1995), 24(1), 111-23
CODEN: BFSAE6; ISSN: 1010-2671

Assiut University

DT Journal

PB

LA English

AB Reaction of Et p-(2-benzimidazolyl)phenoxyacetate (1) with aromatic amines gave the corresponding acetanilides. Reaction of 1 with hydrazine hydrate gave the hydrazide, which reacted with aromatic aldehydes, acetylacetone, Et acetoacetate, CS2, etc. Antibacterial activity of several derivs. was determined

IT 175028-45-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis and antimicrobial activities of benzimidazole derivs.)

RN 175028-45-2 HCAPLUS

CN Acetic acid, [4-(1H-benzimidazol-2-yl)phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 10 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:612183 HCAPLUS

DN 123:198653

TI Synthesis of some 1,3,4-oxadiazolines and thiazolidinones of expected antibacterial activity

AU Abbas, Safinaz E.; El Ansary, Soheir L.; Mikhael, Anwar N.

CS Faculty Pharmacy, Cairo University, Cairo, Egypt

SO Egyptian Journal of Pharmaceutical Sciences (1994), 35(1-6), 21-30

CODEN: EJPSBZ; ISSN: 0301-5068

PB National Information and Documentation Centre

DT Journal

LA English

AB Reaction of the acid hydrazide 4,3,5-ClMe2C6H2OCH2C(0)NHNH2 with different carbonyl compds. gave the corresponding hydrazones 4,3,5-ClMe2C6H2OCH2C(0)NHN:CRR1 [R = H, Me; R1 = CH:CHPh, Me, (un)substituted Ph]. The oxadiazolines were obtained by refluxing the hydrazones with acetic anhydride. The thiazolidinones were achieved by the cyclocondensation of the hydrazones with mercaptoacetic acid. The antimicrobial activity was determined for eight representative compds. and some of them were active.

IT 167995-30-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and antibacterial activity of oxadiazolines and thiazolidinones)

RN 167995-30-4 HCAPLUS

CN Acetic acid, (4-chloro-3,5-dimethylphenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 11 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:96219 HCAPLUS

DN 122:105731

TI Synthesis of some bis-2-azetidinones, bis-4-thiazolidinones and their pharmacological activity

AU Kudari, S. M.; Sajjanshetty, A. S.

CS Dept. of Chemistry, Gulbarga Univ., Karnataka, 585 106, India

SO Oriental Journal of Chemistry (1994), 10(1), 15-18 CODEN: OJCHEG; ISSN: 0970-020X

DT Journal

LA English

GI

AB Condensation of 1,4-bis(hydrazinocarbonylmethoxy)benzene with aromatic aldehydes gave 1,4-bis(arylhydrazinocarbonylmethoxy)benzenes in good yields. These on treatment with chloroacetyl chloride, phenylacetyl chloride and thioglycolic acid gave 1,4-bis[[(3-chloro-4-aryl-2-oxo-1-azetidinyl)amino]ethoxy]benzenes and 1,4-bis[[(4-oxo-3-thiazolidinyl)amino]ethoxy]benzenes I [R = (un)substituted phenyl]. Example compds. are 2,2'-[1,4-phenylenebis(oxy)]bis[N-(1-azetidinyl)acetetamides] and 2,2'-[1,4-phenylenebis(oxy)]bis[N-(3-thiazolidinyl)acetamides]. I were evaluated for diuretic activity against standard drug acetazolamide.

IT 160510-79-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of diuretic [phenylenebis(oxy)]bis[N-azetidinylacetamide]
[phenylenebis(oxy)]bis[N-thiazolidinylacetamide])

RN 160510-79-2 HCAPLUS

CN Acetic acid, 2,2'-[1,4-phenylenebis(oxy)]bis-,
bis[(phenylmethylene)hydrazide] (9CI) (CA INDEX NAME)

L58 ANSWER 12 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:508684 HCAPLUS

DN 121:108684

TI Synthesis of quinazolinyl-benzylidene methyl benzylidene hydrazides as CNS active and antiinflammatory agents

AU Mohan, Rajiv Ravindra

CS Dep. Chem., R.B.S. Coll., Agra, India

SO Journal of Indian Council of Chemists (1993), 9(1), 40-4 CODEN: JICCE7; ISSN: 0971-5037

DT Journal

LA English

GI

AB A series of twenty-four new hydrazides [I, R = Me, Et; R2R2 = CR1C6H4X (R1 = H, Me; X = 2-OH, 4-NH2, etc.)] have been synthesized by the condensation of I (same R; R2 = H) with XC6H4COR1. All the compds. were found to be nontoxic and CNS stimulants (24-53%) or depressants (28-48%). Most of the tested compds. showed significant carrageenin induced mice paw edema

Ι

(20-48%) antiinflammatory activity.

IT 156601-30-8P 156601-42-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and CNS activity and antiinflammatory activity of)

RN 156601-30-8 HCAPLUS

CN Acetic acid, [(2-methyl-4-quinazolinyl)oxy]-, [[4-[2-oxo-2-[(phenylmethylene)hydrazino]ethoxy]phenyl]methylene]hydrazide (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 156601-42-2 HCAPLUS

CN Acetic acid, [(2-ethyl-4-quinazolinyl)oxy]-, [[4-[2-oxo-2-[(phenylmethylene)hydrazino]ethoxy]phenyl]methylene]hydrazide (9CI) (CAINDEX NAME)

PAGE 1-A

PAGE 2-A

L58 ANSWER 13 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:106490 HCAPLUS

DN 120:106490

TI Studies on synthesis and antimicrobial evaluation of some new thiophenol derivatives

AU Bhatt, K. N.; Dave, A. M.; Desai, N. C.; Undavia, N. K.; Trivedi, P. B.

CS Univ. Dep. Chem., Bhavnagar Univ., Bhavnagar, 364 002, India

SO Journal of the Indian Chemical Society (1992), 69(11), 785-7 CODEN: JICSAH; ISSN: 0019-4522

DT Journal

LA English

OS CASREACT 120:106490

GI

Condensation reactions of PhSCH2CONHNH2 (I) with aromatic aldehydes gave the Schiff base derivative which on cycloaddn. with mercaptoacetic acid in dioxane gave 2-aryl-3-(phenylthioacetamido)-4-thiazolidinones [II; R = H, 2-HO, 3,4-(MeO)2, etc.]. 4-(Aryl)-1-phenylthioacetyl-3-thiosemicarbazides III (R = H, 2-, 3-, 4-Me, 2-, 3-, 4-MeO, 2-, 3-, 4-Cl) were prepared by reaction of aryl isothiocyanates with I in boiling EtoH. I easily underwent reaction with aromatic cyanohydrins to give α - (phenylthioacetylhydrazino)arylacetonitriles IV [R = H, 3-NO2, 4-Me, 4-OH, 3,4-(MeO)2, etc.]. Derivs. II-IV exhibited moderate antibacterial activity.

IT 152489-26-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cycloaddn. with mercaptoacetic acid)

RN 152489-26-4 HCAPLUS

CN Acetic acid, (phenylthio) -, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

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L58
    ANSWER 14 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     1993:560167 HCAPLUS
DN
     119:160167
TI
     4-Thiazolidinones. Part II: 2-Aryl-3-(2'-isopropyl-5'-
     methylphenoxyacetylamino) -5-carboxymethyl-4-thiazolidinones
     Roda, K. P.; Vansdadia, R. N.; Parekh, Hansa
AU
CS
     Chem. Dep., Saurashtra Univ., Rajkot, 360 005, India
SO
     Journal of the Institution of Chemists (India) (1992), 64(3),
     109-11
     CODEN: JOICA7; ISSN: 0020-3254
DT
     Journal
LA
     English
GI
```

AB 4-Thiazolidinones I (R = aryl) were prepared by condensation of 2-isopropyl-5-methylphenoxyacetic acid hydrazide, prepared from thymol acetate and N2H4, with RCHO to give the corresponding Schiff bases which were cyclocondensed with HO2CCH(SH)CH2CO2H. All I were active against Salmonella typhosa and had some activity against other Gram-pos. and Gram-neq. bacteria.

IT 111303-67-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and cyclocondensation with thiomalic acid, thiazolidinones
 from)

RN 111303-67-4 HCAPLUS

CN Acetic acid, [5-methyl-2-(1-methylethyl)phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 15 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:472327 HCAPLUS

DN 119:72327

TI Synthesis and antibacterial study of metal complex of 1-(2,4-dichlorophenoxyacetyl)-2-(2-hydroxybenzylidene/naphthylidene)]hydrazine

AU Oza, S. P.; Dave, M. P.; Patel, R. S.

CS Vilco Lab. (P) Ltd., Bhavnagar, India

SO Indian Drugs (1993), 30(1), 48-52 CODEN: INDRBA; ISSN: 0019-462X

DT Journal

LA English

AB The title ligands 2,4-Cl2C6H3OCH2CONHN:CR (R = o-HOC6H4, 2-hydroxynaphthyl) were prepared via 4 steps starting from 2,4-Cl2C6H3OH. Their Cu, Co, Ni and Zn complexes were prepared Test data were given for the antibacterial properties of the ligands and metal complexes against S. aureus and E. coli.

IT 2496-37-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with metal salts)

RN 2496-37-9 HCAPLUS

CN Acetic acid, (2,4-dichlorophenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 16 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:101881 HCAPLUS

DN 118:101881

TI Synthesis of certain 1,3,4-oxadiazole derivatives of expected antiinflammatory activity

AU Abbas, S. E.; Abou-Youssef, H. E.; El-Taliawi, G. M.; Hassan, A. B.

CS Fac. Pharm:, Cairo Univ., Cairo, Egypt

SO Egyptian Journal of Pharmaceutical Sciences (1991), 32(3-4), 515-27

CODEN: EJPSBZ; ISSN: 0301-5068

DT Journal

LA English

OS CASREACT 118:101881

GΙ

$$CH_{2}CONHN = C R$$

$$R_{1}$$

$$CH_{2}CONHN = C R$$

$$R_{1}$$

$$CH_{2}CONHN = C R$$

$$R_{1}$$

$$CH_{2}CH_{2}$$

$$R_{1}$$

$$CH_{2}CH_{2}$$

$$R_{1}$$

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$$CH_{2}CH_{2}$$

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The synthesis of certain diclofenac acid hydrazones I [R = H, R1 = CH:CHPh, 4-MeOC6H4, 2-HoC6H4, 4-Ho-3-MeOC6H3, 4-Me2NC6H4; R = Me, R1 = Me, Et, Ph, 4-MeC6H4, 4-BrC6H4; RR1 = (CH2)5] is described. The A2-1,3,4-oxadiazoline-5-thione II (R2 = H) is prepared by reacting diclofenac acid hydrazide with carbon disulfide in ethanolic potassium hydroxide. Some thioethers, II (R2 = Me, Et, allyl, Bu, CH2CONHPh, CH2CONHC4H4OMe-4), and Mannich bases, III (R3 = pyrrolidinyl morpholinyl, N-methylaniline, dibenzylamino, dimethylamino, diethylamino), were prepared from the 1,3,4-oxadiazole derivative II (R2 = H) and tested for their analgetic, antipyretic, and antiinflammatory activities.

IT 145262-72-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(antiinflammatory, analgesic, and antipyretic activity of)
145262-72-2 HCAPLUS
Benzeneacetic acid, 2-[(2,6-dichlorophenyl)amino]-, [(2-hydroxyphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN

CN

GI

L58 ANSWER 17 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1992:106155 HCAPLUS DN 116:106155 ΤI Synthesis of thiazolidine-containing benzylidene/methylbenzylidenehydrazides and their Mannich bases as CNS active and antiinflammatory agents AU Mohan, Rajiv Ravindra CS Dep. Chem., RBS Coll., Agra, 282 002, India SO Indian Drugs (1991), 29(3), 120-2 CODEN: INDRBA; ISSN: 0019-462X DTJournal LA English

$$R^{2}N$$
 S
 CH
 $OCH_{2}CONHN = CR$
 R^{1}

AB Title compds. I (R = H, Me; R1 = H, 2-OH, 4-OH, 4-OMe, 4-Me, etc.; R2 = H) were prepared from [[α -(5-oxo-2-thioxo-4-thiazolidinylidene)tolyl]oxy] acetic acid hydrazide and benzaldehydes or acetophenones and were subjected to Mannich reactions with HCHO and anilines to give I (same R, R1; R2 = substituted anilinomethyl). Several of the compds. showed CNS activity and were muscle relaxants and antiinflammatants.

IT 139298-28-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, Mannich reaction and biol. activity of)

RN 139298-28-5 HCAPLUS

CN Acetic acid, [4-[(4-oxo-2-thioxo-5-thiazolidinylidene)methyl]phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 18 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1992:41029 HCAPLUS DN 116:41029 ΤI Some sulfonamide derivatives and their antimicrobial activity ΑU Ismail, I. Imam; Mandour, A.; Abd El-Aleem, A. H. CS Fac. Sci., Menoufia Univ., Egypt SO Delta Journal of Science (1989), 13(1), 185-95 CODEN: DJSCES; ISSN: 1012-5965 DT Journal LΑ English

GI

AB Acid hydrazides RCONHNH2 (R = Ph, CH2Ph, 2-MeC6H4, 3-MeC6H4, 4-O2NC6H4, 4-pyridyl) react with 4-H2NC6H4COMe to give RCONHN:CMeC6H4NHR1-4 (I, R1 = H). I (R1 = H) condense with ClSO2C6H4NHCOMe-4 to give I (R1 = SO2C6H4NHCOMe-4) (II) which undergo hydrolysis to give I (R1 = SO2C6H4NH2) (III). I (R1 = H) also react with sultones IV and V to give cyclic sulfonamides VI and I [R1 = (CH2)3SO3H] (VII), resp. Bactericidal and fungicidal activities of I (R1 = H), II, III, VI, and VII were measured. IT 138225-27-1P 138225-28-2P 138225-33-9P 138225-34-0P 138225-39-5P 138225-40-8P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, bactericidal, and fungicidal activity of) RN138225-27-1 HCAPLUS Benzoic acid, 2-methyl-, [1-[4-[[(4-aminophenyl)sulfonyl]amino]phenyl]ethy CN

VΙ

lidene]hydrazide (9CI) (CA INDEX NAME)

RN 138225-28-2 HCAPLUS

CN Benzoic acid, 3-methyl-, [1-[4-[[(4-aminophenyl)sulfonyl]amino]phenyl]ethy lidene]hydrazide (9CI) (CA INDEX NAME)

RN 138225-33-9 HCAPLUS

CN Benzoic acid, 2-methyl-, [1-[4-(3,5-dimethyl-1,1-dioxido-2H-1,2-thiazin-2-yl)phenyl]ethylidene]hydrazide (9CI) (CA INDEX NAME)

RN 138225-34-0 HCAPLUS

CN Benzoic acid, 3-methyl-, [1-[4-(3,5-dimethyl-1,1-dioxido-2H-1,2-thiazin-2-yl)phenyl]ethylidene]hydrazide (9CI) (CA INDEX NAME)

RN 138225-39-5 HCAPLUS

CN Benzoic acid, 2-methyl-, [1-[4-[(3-sulfopropyl)amino]phenyl]ethylidene]hyd
razide (9CI) (CA INDEX NAME)

RN 138225-40-8 HCAPLUS

CN Benzoic acid, 3-methyl-, [1-[4-[(3-sulfopropyl)amino]phenyl]ethylidene]hyd
razide (9CI) (CA INDEX NAME)

$$HO_3S-(CH_2)_3-NH$$
 Me
 $C=N-NH-C$

IT 138225-21-5P 138225-22-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, hydrolysis, fungicidal, and bactericidal activity of)

RN 138225-21-5 HCAPLUS

CN Benzoic acid, 2-methyl-, [1-[4-[[[4-(acetylamino)phenyl]sulfonyl]amino]phenyl]ethylidene]hydrazide (9CI) (CA INDEX NAME)

RN 138225-22-6 HCAPLUS

CN Benzoic acid, 3-methyl-, [1-[4-[[[4-(acetylamino)phenyl]sulfonyl]amino]phenyl]ethylidene]hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 19 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:206680 HCAPLUS

DN 114:206680

TI Antihypertensive hydrazidones: study of acylated 2-chlorobenzylidenehydrazines

AU Galons, H.; Cave, C.; Miocque, M.; Rinjard, P.; Tran, G.; Binet, P.

CS Lab. Chim. Org., Fac. Pharm., Chatenay-Malabry, F 92290, Fr.

SO European Journal of Medicinal Chemistry (1990), 25(9), 785-8 CODEN: EJMCA5; ISSN: 0223-5234

DT Journal

LA French

OS CASREACT 114:206680

GI

AB Fifty-five hydrazones I (R = H, Me, Et, Bu, CH2OH; R1 = CMe2OH, 3,4,5-trimethoxyphenyl, CONH2, 3-pyridyl, etc.) were prepared from the carbonyl compds. and the acylhydrazines. Antihypertensive min. dosage for I in rats are tabulated.

IT 133661-81-1P 133662-86-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and antihypertensive activity of)

RN 133661-81-1 HCAPLUS

CN Benzeneacetic acid, 4-methoxy-, [(2-chlorophenyl)methylene]hydrazide, (E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

Ι

RN 133662-86-9 HCAPLUS

CN Benzeneacetic acid, 4-methoxy-, [(2-chlorophenyl)methylene]hydrazide, (Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

L58 ANSWER 20 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:143256 HCAPLUS

DN 114:143256

TI Synthesis and antiinflammatory activity of benzal-3pentadecylaryloxyalkylcarboxylic acid hydrazides and 2-benzalamino-5-(3'pentadecylaryloxyalkyl)-1,3,4-oxadiazoles

AU Ramalingam, T.; Sattur, P. B.

CS Indian Inst. Chem. Technol., Hyderabad, 500 007, India

European Journal of Medicinal Chemistry (1990), 25(6), 541-4

Ι

CODEN: EJMCA5; ISSN: 0223-5234

DT Journal LA English

LA GI

SO

OCHR¹CONHN=CH
$$R^2$$
R4

(CH₂) 14Me

$$\begin{array}{c}
N-N \\
OCHR^{1} \longrightarrow N = CH \longrightarrow OMe
\end{array}$$

$$\begin{array}{c}
(CH_{2})_{14}Me
\end{array}$$

AB Hydrazides I (R = H, Cl; R1 = H, Me; R2 = H, OH, NO2, Cl; R3 = H, MeO; R4 = H, Cl, MeO, OCH2CO2H) and oxadiazoles II (R = H, Cl; R1 = H, Me) were prepared in 48-96% yields by, e.g., condensing m-Me(CH2)14C6H4OCH2CONHNH2 with BzH, and their antiinflammatory activity tested by the carrageenin-induced rat paw edema method.

II

IT 132663-55-9P 132663-61-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antiinflammatory activity of)

RN 132663-55-9 HCAPLUS

RN 132663-61-7 HCAPLUS

L58 ANSWER 21 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:70043 HCAPLUS

DN 114:70043

TI Stoichiometric stability constants of complexes with bioactive hydrazide-type ligands

AU Tschwatschal, Frank; Dietze, Frank; Seidel, Andreas; Thomas, Philipp

CS Sekt. Chem., Karl-Mark-Univ., Leipzig, DDR-7010, Ger. Dem. Rep.

SO Zeitschrift fuer Chemie (1990), 30(9), 331-2 CODEN: ZECEAL; ISSN: 0044-2402

DT Journal

LA German

AB Complexation of Cu2+, Ni2+, Zn2+, Co2+, Mn2+, or Pb2+ with MeSC(S)NHN:CRR1 or 2,4-C6H3Cl2OCH2C(O)NHN:CRR1 (R = H, Me; R1 = Ph, 2-pyridyl, 2-furyl, 2-hydroxyphenyl, COOH) was studied pH-metrically and spectrophotometrically at 298 K in 75 volume % aqueous dioxane (ionic strength 0.1 (Me4NNO3)). Successive stability consts. were calculated by using the MINIQUAD (P. Gaus et al. 1976) program.

IT 2496-37-9

RL: PEP (Physical, engineering or chemical process); PROC (Process) (ionization of, in aqueous dioxane)

RN 2496-37-9 HCAPLUS

CN Acetic acid, (2,4-dichlorophenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 22 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:590989 HCAPLUS

DN 113:190989

TI Studies on 2-azetidinones. Part-I. Preparation and antimicrobial activity of p,p'-bis(3-chloro-4-aryl-2-azetidinon-l-ylcarbamoylmethoxy)diphenyl sulfones

AU Vansdadia, R. N.; Roda, K. P.; Parekh, Hansa

CS Dep. Chem., Saurashtra Univ., Rajkot, 360 005, India

SO Journal of the Indian Chemical Society (1989), 66(1), 56-8 CODEN: JICSAH; ISSN: 0019-4522

DT Journal

LA English

OS CASREACT 113:190989

$$\begin{bmatrix} R & NNHCOCH_2O & \\ C1 & O & \\ \end{bmatrix}_2^{SO_2}$$

AB Azetidinones I (R = Ph, substituted Ph) were prepared by treatment of (4-EtO2CCh2OC6H4)2SO2 with N2H4, treatment of the dihydrazide with RCHO, and cyclization of the dihydrazones with ClCH2Cl. Maximum fungicidal activity (≤ 20 mm inhibition zone) was observed in I [R = 4-ClC6H4, 3,2-MeO(HO)C6H3, 4-HOC6H4] against Aspergillus niger and in I (R = 2-O2NC6H4) against Saccharomyces cerevisiae. I [R = 2,6-Cl2C6H3, 3,2-MeO(OH)C6H3] had maximum activity against Serrati marescens.

RN 123798-85-6 HCAPLUS

CN Acetic acid, 2,2'-[sulfonylbis(4,1-phenyleneoxy)]bis-, bis[(phenylmethylene)hydrazide] (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

— Ph

L58 ANSWER 23 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:77018 HCAPLUS

DN 112:77018

TI Studies on 4-thiazolidinones. Part IX. Preparation and antimicrobial activity of p,p'-bis(2-aryl-5H/methyl-4-thiazolidinon-3-ylmethoxy)diphenyl sulfones

AU Vansdadia, R. N.; Roda, K. P.; Parekh, Hansa

CS Dep. Chem., Saurashtra Univ., Rajkot, 360 005, India

SO Journal of the Indian Chemical Society (1989), 66(2), 113-15 CODEN: JICSAH; ISSN: 0019-4522

DT Journal

LA English

OS CASREACT 112:77018

AB Hydrazinolysis of O2S(C6H4OCH2COR-4)2 (I, R = OEt) in EtOH gave 87% I (R = NHNH2) which on condensation with R1CHO [R1 = (un)substituted phenyl] gave 59-80% Schiff bases I (R = NHN:CHR1) (II). Cyclization of II with HSCHR2CO2H (R2 = H, Me) gave 59-85% title compds. III.

IT 123798-85-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation of, with thioglycolic or thiolactic acids, thiazolidinone derivs. by)

RN 123798-85-6 HCAPLUS

CN Acetic acid, 2,2'-[sulfonylbis(4,1-phenyleneoxy)]bis-,
bis[(phenylmethylene)hydrazide] (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

-- Ph

L58 ANSWER 24 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1989:632632 HCAPLUS DN 111:232632 TI 4-Thiazolidinones. Part VII. Preparation and antimicrobial activity of p,p'-bis(2-aryl-5-carboxymethyl-4-thiazolidinon-3ylcarbamoylmethoxy)diphenyl sulfones ΑU Vansdadia, R. N.; Roda, K. P.; Parekh, Hansa CS Dep. Chem., Saurashtra Univ., Rajkot, 360 005, India SO Journal of the Institution of Chemists (India) (1988), 60(5), 191-3 CODEN: JOICA7; ISSN: 0020-3254 DT Journal LA English os CASREACT 111:232632

AB Twenty title compds. I (R = Ph, substituted Ph) were prepared by the cyclocondensation of 4-[RCH:NNHCOCH2OC6H4]2SO2 with thiomalic acid. I were tested for antimicrobial activity against Staphylococcus aureus, Staphylococcus citrus, Escherichia coli, Marcsane serratia, Saccharomyces cerevisiae, and Aspergillus niger and showed good activity.

IT 123798-85-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and cyclocondensation reaction with thiomalic acid)

RN 123798-85-6 HCAPLUS

CN Acetic acid, 2,2'-[sulfonylbis(4,1-phenyleneoxy)]bis-, bis[(phenylmethylene)hydrazide] (9CI) (CA INDEX NAME)

I

PAGE 1-A

PAGE 1-B

— Ph

ANSWER 25 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN L58 1989:497182 HCAPLUS ANDN111:97182 New 4-quinazolinones as antibacterial agents TI ΑU Sakr, S. M.; El-Sadek, M.; Al-Ashmawi, M. I. CS Fac. Pharm., Zagazig Univ., Egypt SO Egyptian Journal of Pharmaceutical Sciences (1988), 29(1-4), 243-50 CODEN: EJPSBZ; ISSN: 0301-5068 DT Journal LA English os CASREACT 111:97182

Ι

ΙI

AB The [(hydrazinocarbonylmethoxy)phenyl]quinazolinones I [R = R1 = Me, R = H, Me, R1 = (un)substituted phenyl] were prepared by treating 3-(4-hydroxyphenyl)-2-methyl-7-nitro-4(3H)-quinazolinone with ClCH2CO2Et followed by H2NNH2.H2O and then RCOR1. Some I were cyclized by treatment with Ac2O to give the oxadiazole derivs. II. Some I and II were screened for antibacterial activity.

IT 120984-92-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and intramol. cyclization of)

RN 120984-92-1 HCAPLUS

CN Acetic acid, [4-(2-methyl-7-nitro-4-oxo-3(4H)-quinazolinyl)phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 26 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1987:119744 HCAPLUS

DN 106:119744

TI Synthesis of some important 4-thiazolidinones as potential tuberculostatic and antibacterial agents. Part I

AU Shah, S. R.; Gol, D. D.; Shah, S. J.; Thaker, K. A.

CS Dep. Chem., Bhavnagar Univ., Bhavnagar, 364 002, India

SO Journal of the Institution of Chemists (India) (1986), 58(1), 10-12

CODEN: JOICA7; ISSN: 0020-3254

DT Journal

LA English

OS CASREACT 106:119744

GΙ

$$C1$$
 OCH₂CONH-N-S

AB Thiazolidinones I (R = H, CH2CO2H; R1 = Ph, substituted Ph) were preped. by the cyclocondensation of 4-ClC6H4OCH2CONHN:CHR1 with RCH(SH)CO2H. I showed tuberculostatic activity in vitro, at various concns.; I (R1 = 2-ClC6H4) were most active. They showed little or moderate antibacterial activity at high concns.

IT 2503-75-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation with mercapto acids)

Ι

RN 2503-75-5 HCAPLUS

CN Acetic acid, (4-chlorophenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 27 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1987:102148 HCAPLUS

DN 106:102148

TI Synthesis of some newer 4-(3-methyl-5-oxo-4-pyrazolidinylidenemethyl)pheno xyacetic acid benzylidenehydrazides and α -methylbenzylidenehydrazides as CNS active and antiinflammatory agents

AU Mohan, Rajiv Ravindra; Agarwal, Chapla; Misra, V. S.

CS Dep. Chem., Univ. Lucknow, Lucknow, 226 007, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1986), 25B(3), 339-41 CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

OS CASREACT 106:102148

CH—CH2CONHNH2

AB The title compds. I (R = H, Me; R1 = Ph, substituted phenyl) were prepared by condensation of hydrazides II with RCOR2. II was prepared by condensation of 3-methyl-5-oxopyrazole with p-OHCC6H4OCH2CO2Et followed by treatment with H2NNH2.H2O. I had central nervous systems stimulant or depressant activity and gave 4-23% protection against carrageenin-induced mice paw edema.

Ι

II

IT 107044-90-6P

RN

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and central nervous system and antiinflammatory activity of) 107044-90-6 HCAPLUS

CN Acetic acid, [4-[(1,5-dihydro-3-methyl-5-oxo-4H-pyrazol-4-ylidene)methyl]phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 28 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1986:549243 HCAPLUS

DN 105:149243

TI Preparation of protein conjugates via intermolecular hydrazone linkage

AU King, Te Piao; Zhao, Shu Wei; Lam, Terence

CS Rockefeller Univ., New York, NY, 10021-6399, USA

SO Biochemistry (1986), 25(19), 5774-9 CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

AB Proteins can be modified at their amino groups under gentle conditions to produce derivs. containing an average of 3-6 aryl aldehyde or acyl hydrazide

groups. These 2 types of modified proteins at .apprx.10 μM concentration condense with each other at pH .apprx.5 to form conjugates linked by hydrazone bonds. Under proper conditions, conjugates containing mainly dimers and trimers or, if desired, higher oligomers can be obtained. The conjugates can be dissociated to their individual protein components by an exchange reaction with an excess of acetyl hydrazide. The reversible hydrazone bonds of conjugates can be reduced with NaCNBH3 to give stable hydrazide bonds. The stability of protein-hydrazone conjugates was significantly greater than that of the model compound, the N-acetylhydrazone of p-carboxybenzaldehyde. This difference is believed to result from the presence of multiple hydrazone linkages in protein conjugates.

IT 25996-47-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and UV spectrum of)

RN 25996-47-8 HCAPLUS

CN Acetic acid, [(4-nitrophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 29 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1985:184999 HCAPLUS

DN 102:184999

TI Studies on 4-thiazolidinones as antibacterial agents

AU Shah, S. J.; Shah, S. R.; Desai, N. C.; Thaker, K. A.

CS Dep. Chem., Bhavnagar Univ., Bhavnagar, 364 002, India

SO Journal of the Indian Chemical Society (1984), 61(7), 648-9 CODEN: JICSAH; ISSN: 0019-4522

DT Journal

LA English

OS CASREACT 102:184999

GI

AB Bactericidal thiazolidinones I (R = Ph, substituted Ph, R1 = H, CH2CO2H) were prepared in 55-60% yields by cyclocondensation of PhCH2CONHN:CHR, prepared in 65-75% yields by condensation of RCHO with PhCH2CONHNH2, with R1CH(SH)CO2H. I (R = 5,2-Br(HO)C6H2, R1 = H) inhibited Staphylococcus aureus in an agar plate test to give a zone diameter >20%.

IT 1087-36-1P 54009-60-8P 67759-87-9P 92965-60-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and cyclocondensation with thioglycolic and thiomalic acids)

RN 1087-36-1 HCAPLUS

CN Benzeneacetic acid, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

RN 54009-60-8 HCAPLUS

CN Benzeneacetic acid, [(2-hydroxyphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 67759-87-9 HCAPLUS

CN Benzeneacetic acid, [(4-chlorophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

RN 92965-60-1 HCAPLUS

CN Benzeneacetic acid, [(4-methylphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

$$CH = N - NH - C - CH_2 - Ph$$

L58 ANSWER 30 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1985:24441 HCAPLUS

DN 102:24441

TI Synthesis and antifungal activity of some new 2[2-(4'-aryl-5'-methoxystyryl)-1',2',4'-triazol-3'-thiol]pyridines [4-aryl-5-[2-[2-(2-pyridyl)vinyl]phenoxy]methyl-1,2,4-triazole-3-thiones]

AU Bhattacharya, B. K.; Dirk, V. D.; Hoornaert, G.; Sawant, S.

CS Dep. Chem., Polytech. Inst. New York, Brooklyn, NY, 11201, USA

SO Bokin Bobai (1984), 12(8), 383-90 CODEN: BOBODP; ISSN: 0385-5201

DT Journal

LA English

$$CH = CH - CH = CH - CONHR$$
 I

$$\begin{array}{c|c} & & \\ \hline \\ N \end{array} \begin{array}{c} \text{CH} = \text{CH} \\ \hline \\ \text{OCH}_2 \end{array} \begin{array}{c} N - NR^2 \\ \hline \\ R^1 \end{array} \begin{array}{c} \text{II} \end{array}$$

The hydrazide I (R = NH2) on treatment with R1NCS (R1 = Ph, substituted Ph, 2-furyl) furnished I (R = NHCS2NHR1) which on cyclization with NaOH yielded the triazolethiols II (R2 = H). On treatment with R3COCl (R3 = Ph, C16H4, 2,4-C12C6H3) II (R2 = H) yielded II (R2 = COR3). Sixteen of these compds. were screened for their fungicidal activity against Aspergillus niger and Aspergillus flavus compared with Benomyl, structure activity relationship are discussed.

IT 93912-06-2P

RN 93912-06-2 HCAPLUS

CN Acetic acid, [2-[2-(2-pyridinyl)ethenyl]phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 31 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1981:619992 HCAPLUS

DN 95:219992

TI Synthesis of ethyl p-(2-benzoxazolyl)phenoxyacetate and corresponding hydrazides

AU Bahadur, Surendra; Pandey, K. K.

CS Chem. Dep., Lucknow Univ., Lucknow, 226 007, India

SO Journal of the Indian Chemical Society (1981), 58(9), 883-4 CODEN: JICSAH; ISSN: 0019-4522

DT Journal

LA English

OS CASREACT 95:219992

AB Etherification of benzoxazole I (R = H) with ClCH2CO2Et gave I (R = CH2CO2Et), which was treated with N2H4 to give I (R = CH2CONHNH2) (II). Condensation of II with R1CHO (R1 = Ph, 4-ClC6H4, 4-O2NC6H4, 4-HOC6H4, 2-HOC6H4, 2,3-HO(MeO)C6H3, 4-MeOC6H4, 2-furyl) gave I (R = OCH2CONHN:CHR1) (III), reduction of which with NaBH4 gave I (R = OCH2CONHNHCH2R1 (IV). Antiviral and bactericidal activity of III and IV was given.

IT 79945-53-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and bactericidal activity of)

RN 79945-53-2 HCAPLUS

CN Acetic acid, [4-(2-benzoxazolyl)phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 32 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1977:155582 HCAPLUS

DN 86:155582

TI Synthesis of a few acid hydrazides: sulfonyl hydrazides and their derivatives from 2-phenyl-1,2,3-triazole-4-carboxylic acid and [(4-nitrophenyl)thio]acetic acid as antibacterials

AU Nadkarny, V. V.; Rao, R. S.; Fernandes, P. S.

CS Nadkarny-Sacasa Res. Lab., St. Xavier's Coll., Bombay, India

SO Journal of the Indian Chemical Society (1976), 53(8), 833-6 CODEN: JICSAH; ISSN: 0019-4522

DT Journal

LA English

GI

$$R^{1}$$
 I, R=CONHN:CHR², R¹=H II, R=CO₂H, R¹=SO₂NHN:CHR²

AB The triazoles I and II and p-O2NC6H4SCH2CONHN: CHR2 (R2 = 2-furyl, C6H4R3, R3 = H, NO2-p, OH-o, OMe-p) were prepared by treating OCHR2 with the corresponding acid hydrazides, which inhibited the growth of Staphylococcus aureus, Escherichia coli, and Salmonella typhi.

IT 62352-45-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 62352-45-8 HCAPLUS

CN Acetic acid, [(4-nitrophenyl)thio]-, (phenylmethylene)hydrazide (9CI) (CA

INDEX NAME)

L58 ANSWER 33 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1976:508377 HCAPLUS

DN 85:108377

TI Synthesis of some p-sec-amyl phenoxyacetyl hydrazones and their antibacterial activity

Ι

AU Sen Gupta, Anil K.; Avasthi, Kamlakar; Imam, S. A.

CS Dep. Chem., Univ. Lucknow, Lucknow, India

SO Indian Journal of Pharmacy (1976), 38(1), 11-12 CODEN: IJPAAO; ISSN: 0019-5472

DT Journal

LA English

GΙ

AB Benzaldehydes and PhCH:CHCHO condensed with a phenoxyacetohydrazide derivative to give eighteen hydrazones I (R = Ph, substituted phenyl, PhCH:CH) which showed bactericidal activity.

IT 60219-70-7P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and bactericidal activity of)

RN 60219-70-7 HCAPLUS

CN Acetic acid, (4-sec-pentylphenoxy)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 34 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1974:413235 HCAPLUS

DN 81:13235

TI Preparation of hydrazide derivatives of phenoxyacetic acid. In vitro study of its monoamine oxidase inhibiting activity. II. Azote substitution derivatives

AU Orzalesi, H.; Castel, J.; Fulcrand, P.; Chevallet, P.; Soulas, D.; Noel,

A. M.

CS Lab. Pharm. Chim., Fac. Pharm., Montpellier, Fr.

SO Travaux de la Societe de Pharmacie de Montpellier (1974), 33(4), 623-8

CODEN: TSPMA6; ISSN: 0037-9115

DT Journal

LA French

The condensation of PhOCH2CONHNH2 with aldehydes and ketones gave PhOCH2CONHN:CRR1 which were converted to five PhOCH2-CONHNHCHRR1 (I; R = H, Me; R1 = Me, Ph, PhCH2, CO2H). Hydrazines and PhOCH2CO2Et gave PhOCH2CON-HNHR (II; R = Me, Ph). I and II are potential monoamine oxidase inhibitors.

IT 52093-72-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrogenation of)

RN 52093-72-8 HCAPLUS

CN Acetic acid, phenoxy-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 35 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1973:427830 HCAPLUS

DN 79:27830

TI Mutagenic effect of new chemical compounds. II. Mutagenic effect of phenyl- and phenoxyacetic acid derivatives

AU Paronikyan, G. M.; Akopyan, L. G.

CS Inst. Fine Org. Chem., Erevan, USSR

SO Genetika (Moscow) (1973), 9(4), 78-84 CODEN: GNKAA5; ISSN: 0016-6758

DT Journal

LA Russian

AB Of 45 phenylacetic and phenoxyacetic acid ester derivs. tested, 12 were mutagenic toward mutants of Escherichia coli, Actinomyces rimosus, and Saccharomyces cerevisiae. The most active of these was Me 2-chloromethyl-4-bromophenoxy acetate hexamethylenetetramine salt [16253-49-9]. It induced reversion mutants in the threonine and lysine loci in the bacteria.

IT 42024-65-7 42024-69-1 42024-73-7

42024-77-1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(mutagenic activity of)

RN 42024-65-7 HCAPLUS

CN Acetic acid, [4-bromo-2-[(dimethylamino)methyl]phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

CN Acetic acid, [4-bromo-2-[(diethylamino)methyl]phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Br} \\ \\ \text{O} \\ \\ \text{Ph-CH} = \text{N-NH-C-CH}_2 - \text{O} \end{array}$$

RN 42024-73-7 HCAPLUS

RN 42024-77-1 HCAPLUS

CN Acetic acid, [4-bromo-2-(1-piperidinylmethyl)phenoxy]-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

L58 ANSWER 36 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1969:114824 HCAPLUS

DN 70:114824

TI Antiadrenergic and antiarrhythmic 1-aminomethyl-2-phenoxyethanols

IN Wooldridge, Kenneth R. H.; Basil, Berkeley

PA May and Baker Ltd.

SO S. African, 52 pp.

CODEN: SFXXAB

DT Patent

LA English

FAN.CNT 2

111	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PΙ	ZA 6803130	A	19681021	ZA 1968-3130	19680515 <
	GB 1231783	A	19710512	GB 1967-22735	19670516 <
	BE 715205	A	19681118	BE 1968-715205	19680515 <
	FR 1570087	Α	19690606	FR 1968-151931	19680515 <
	FR 7616	M	19700119	FR 1968-151932	19680515 <
	CH 485663	Α	19700215	CH 1969-19428	19680516 <
	CH 489467	Α	19700430	CH 1968-7226	19680516 <

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DE 1768468
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     SU 931103
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                                19820523
                                            SU 1968-1290765
                                                                   19681218 <--
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                                19700115 CH 1968-19020
                                                                   19681220 <--
PRAI GB 1967-58516
                        Α
                                19671222 <--
     GB 1967-22735
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                                19670516 <--
     GB 1968-56513
                        Α
                                19680514 <--
     ZA 1968-3130
                                19680515 <--
     GB 1968-1968
                                19680802 <--
     GB 1968-37103
                         Α
                                19680802 <--
     For diagram(s), see printed CA Issue.
GT
AB
     The title compds. antagonize some effects of adrenaline, noradrenaline,
     and sympathetic stimulation on cardiac muscle, show antiarrhythmic
     properties, and are valuable in treatment of various cardiac disorders
     including coronary disease, angina, and cardiac arrhythmias. Some of them
     posess hypotensive properties. 1-(o-Acetylphenoxy)-2,3-epoxypropane (I)
     (23.6 g.), 8.4 g. NH2OH.-HCl, and 98.5 g. anhydrous NaOAc in 100 cc. dry
     Me2NCHO was stirred for 18 hrs. at room temperature, 50 g. iso-PrNH2 and 50 cc.
     EtOH added, and the mixture refluxed for 3 hrs. to give DL-1-(o-
     acetylphenoxy)-2-hydroxy-3-isopropylaminopropane (II) oxime, m.
     94°. I (15 g.), 15 g. iso-PrNH2, and 25 cc. EtOH was refluxed for
     3 hrs. to give 11 g. II, m. 104-6°, converted conventionally to the
     oxime; II.HCl m. 70-5°. Similarly were prepared DL-2-hydroxy-1-
     isopropylamino-3-(o-propionylphenoxy)propane oxime, m. 68-9°;
     DL-1-(o-butyrylphenoxy)-2-hydroxy-3-isopropyl-aminopropane oxime, m.
     68-70°; DL-2-hydroxy-1-isopropylamino-3-(o-valerylphenoxy)propane
     oxime-HCl, m. 137-8°; DL-2-hydroxy-1-(o-isobutyrylphenoxy)-3-
     isopropylaminopro-pane oxime, m. 64-6°; DL-2-hydroxy-1-
     isopropylamino-3-(o-pivaloylphenoxy)propane oxime-HCl, m. 203-4°;
     DL-1-(o-heptanoylphenoxy)-2-hydroxy-3-isopropylaminopropane oxime-HCl, m.
     107-8°; DL-2-hydroxy-1-(o-isohexanoylphenoxy)-3-iso-
     propylaminopropane oxime-HCl, m. 119-24°; DL-2-hydroxy-1-
     isopropylamino-3-(o-phenylacetylphenoxy)propane oxime, m. 170-2°;
     DL-2-hydroxy-1-isopropylamino-3-[o-(β-phenylpropionyl)phenoxy]propane
     oxime-HCl, m. 150°; DL-2-hydroxy-1-iso-propylamino-3-[o-(4-
     pyridylcarbonyl)phenoxy]propane oxime, m. 120-4°;
     DL-1-(2-acetyl-4-methylphenoxy)-2-hydroxy-3-iso-propylaminopropane oxime,
     m. 97-9°; DL-1-(2-acetyl-4-methoxyphenoxy)-2-hydroxy-3-
     isopropylaminopropane oxime, m. 134-6°; DL-1-(2-acetyl-4-
     chlorophenoxy) -2-hydroxy-3-isopropyl-aminopropane oxime, m.
     104-10°; DL-1-(4-acetamido-2-acetylphenoxy)-2-hydroxy-3-
     isopropylaminopropane oxime, m. 126-9°; DL-1-(2-acetyl-5-
     phenylphenoxy) -2-hydroxy-3-isopropyl-aminopropane oxime, m. 144-6°;
     DL-1-(2-acetyl-3,5-dimethylphenoxy)-2-hydroxy-3-isopropylaminopropane
     oxime, m. 106-10°; DL-1-(2-acetyl-4,5-dimethylphenoxy)-2-hydroxy-3-
     iso-propylaminopropane oxime, m. 127-9°; DL-1-(o-acetylphenoxy)-3-
     tert-butylamino-2-hydroxypropane oxime-2HCl, m. 146-8°;
     DL-1-(o-acetylphenoxy)-3-(2-ethoxyethylamino)-2-hydroxypropane oxime, m.
     79-83°; DL-1-(o-acetylphenoxy)-2-hydroxy-3-isopropylaminopropane
     O-methyloxime HCl salt, m. 142-4°; DL-1-(2-acetyl-4-nitrophenoxy)-2-
     hydroxy-3-isopropylaminopro-pane oxime, m. 155-8°;
     DL-1-(2-acetyl-5-chlorophenoxy)-2-hydroxy-3-isopropylaminopropane oxime,
     m. 119-22°; DL-1-(2-acetyl-4-phenylphenoxy)-2-hydroxy-3-
     isopropylaminopropane oxime, m. 112-15°; DL-1-(2-acetyl-4,5-
     dichlorophenoxy)-3-iso-propylaminopropane oxime, m. 140-2°;
     DL-1-(o-acetylphenoxy)-2-hydroxy-3-(1-methyl-3-phenylpropylamino)propane
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oxime-HCl, m. 139°; and DL-1-(o-acetylphenoxy)-2-hydroxy-3-

isopropyl-aminopropane O-benzyloxime HCl salt, m. 113-14°. The tabulated III were prepared in 2 ways. Method A: A mixture of a phenol, excess epichlorhydrin, K2CO3, and Me2NCHO was heated under N on a steam The period of heating was determined by following the course of the reaction by thin-layer chromatog. The mixture was poured into H2O, extracted with Et20, dried, distilled in vacuo, and recrystd. Method B: The phenol was treated with a solution of EtONa in EtOH, and the precipitated Na salt of the phenol was filtered off and added in portions (sometimes by means of Soxhlet extractor) to a refluxing solution of excess epichlorohydrin in EtOH. mixture was refluxed for a further period (determined by following the course of the reaction by thin-layer chromatoq.) and worked up as in Method A. following intermediates for III were prepared conventionally: o-hydroxypivalophenone, b20 125-35°; 1-(o-hydroxybenzoyl)-3methylbutane, b0.5 115-20°; 1-hydroxy-1-(o-methoxyphenyl)-4methylpentane, b0.5 112-20°; 4-(o-hydroxybenzoyl)pyridine, m. 76-7°; 4-(o-methoxybenzoyl)-pyridine, b0.1 140-50°; 4,5-dichloro-2-hydroxyacetophenone, m. 105-6°. The tabulated IV (R1 = H) were prepared by refluxing III in EtOH with excess amine (method A), carrying out the reaction at room temperature (method B), or heating III and the amine under N at 120° (method C). II (10 g.) was mixed with a solution of 4 g. thiosemicarbazide in 25 cc. H2O and allowed to stand 18 hrs. to give the thiosemicarbazone hydrate, m. 166-8°. Similarly prepared were: II 4-(o-methoxybenzyl)thiosemicarbazone, m. 93-7°; DL-1-(2-acetyl-4-chlorophenoxy)-2-hydroxy-3-isopropyl-aminopropane thiosemicarbazone, m. 100-2°; and DL-1-(2-acetyl-3,5dimethylphenoxy)-2-hydroxy-3-isopropylaminopro-pane thiosemicarbazone, m. 130-2°. Also prepared were II semicarbazone di-HCl salt, m. 159-62°; DL-1-(2-acetyl-4-chlorophenoxy)-2-hydroxy-3isopropylaminopropane semicarbazone, m. 134-5°; DL-1-(2-acetyl-3,5-dimethylphenoxy)-2-hydroxy-3-iso-propylaminopropane semicarbazone, m. 121-4°; DL-1-(2-acetyl-4,5-dimethylphenoxy)-2hydroxy-3-isopropylaminopropane semicarbazone, m. 135-7°; II 4-phenylsemicarbazone di-HCl salt, m. 98-102°; and DL-1-(2-acetyl-4-methoxyphenoxy)-2-hydroxy-3-isopropylaminopropane semicarbazone, m. 128-31°. II (10 g.) in 10 cc. MeOH and 10 cc. 2N AcOH were mixed with 6.45 g. 4-(ethoxyethyl)thiosemicarbazide in 25 cc. 2N AcOH and allowed to stand 30 min. to give II 4-(ethoxyethyl)thiosemicarbazone di-HCl salt, m. 125-8°. Also prepared were II 4-sec-butylthio-semicarbazone di-HCl salt, m. 75-80°; II 4-isobutylthiosemi-carbazone di-HCl salt, m. 151-4°; II 4-tert-butylthiosemicar-bazone di-HCl salt, m. 152-6°; II 4-(o-chlorophenyl)thiosemicarbazone di-HCl salt, m. 125°; II 4-benzylthiosemicarbazone, m. 99-100°; II isonicotinoylhydrazone-3HCl, m. 148-50°; II 4-(2-pyridyl)semicarbazone-HCl, m. 135-6°; DL-1-(o-benzoylphenoxy)-2-hydroxy-3-isopropylaminopropane oxime, m. 122-5°; II 4-methylthiosemicarbazone-2HCl, m. 76°; II hydrazone, m. 96-8°; II p-tolylsulfonylhydrazone, m. 169-72°; II p-methoxyphenylsulfonylhydrazone-HCl, m. 176-7°; II p-nitrophenylsulfonylhydrazone-HCl, m. 176-7°; II p-chloro-phenylsulfonylhydrazone-HCl, m. 181-4°; II m-chlorophenyl sulfonylhydrazone-HCl, m. 168-70°; II 1-naphthylsulfonyl-hydrazone-HCl, m. 122-5°; II 2-naphthylsulfonylhydrazone-HCl, m. 80-2°; II 3-methylisothiazo-4-ylsulfonylhydrazone-2HCl, m. 65-70°; II 4-phenoxyphenylsulfonylhydrazone-2HCl, m. 129-33° (decomposition); II butylsulfonylhydrazone, m. 102-7°; II benzylsulfonylhydrazone, m. 112-17°; II pdimethylaminophenylsulfonylhydrazone-HCl, hydrate, m. 60-80°; II p-cyanophenylsulfonylhydrazone, m. 171-3°; II ochlorophenylsulfonylhydrazone-HCl, m. 183-7°; II

p-bromophenylsulfonylhydrazone-HCl, m. 198-201°; II

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p-acetamidophenylsulfonylhydrazone-HCl, m. 85-7° (decomposition); and II
     p-hydroxyphenylsulfonylhydrazone-HCl, m. 102-7°. The following
     intermediates were prepared conventionally: m-chlorobenzenesulfonyl
     hydrazide, m. 60-4°; p-phenoxybenzene-sulfonyl hydrazide, m.
     137.5-9.5°; p-dimethylaminobenzene-sulfonyl hydrazide hydrate, m.
     230°; and o-chlorobenzenesul-fonyl hydrazide, m. 101-3°.
     DL-1-(4-Chloro-2-propionylphenoxy)-2-hydroxy-3-isopropylaminopropane
     phenylsulfonyl-hydrazone-HCl m. 85-90°. 5'-Chloro-2'-
     hydroxypropiophenone (122 g.) was added to MeONa in MeOH (prepared from 15.5
     g. Na and 1000 cc. anhydrous MeOH) and the mixture concentrated to dryness to
qive
     the Na salt of the phenol. The Na salt was added during 1 hr. to a
     refluxing mixture of 150 cc. epichlorohydrin and 150 cc. MeOH and refluxing
     was maintained for 3 hrs. to give 1-(4-chloro-2-propionylphenoxy)-2,3-
     epoxypropane (V), m. 54°. A mixture of 48 g. V, 100 cc. iso-PrNH2,
     and 100 cc. MeOH was refluxed for 24 hrs. to give DL-1-(4-chloro-2-
     propionylphenoxy) -2-hydroxy-3-isopropylaminopropane, m. 76-81°.
     DL-1-(2-Acetyl-4,6-dichlorophenoxy)-2-hydroxy-3-isopropylaminopropane
     phen-ylsulfonylhydrazone-HCl m. 105-6°. A mixture of 110 g.
     3',5'-dichloro-2'-hydroxyacetophenone, 37.4 g. anhydrous K2CO3, 200 g.
     epichlorohydrin, and 500 cc. anhydrous Me2NCHO was heated under N for 8 hrs.
     at 100° to give 1-(2-acetyl-4,6-dichlorophenoxy)-2,3-epoxypropane,
     b. 140-50°, which (32 g.), 100 cc. iso-PrNH2, and 50 cc. anhydrous
     EtOH was refluxed 7 days to give DL-1-(2-acetyl-4,6-dichlorophenoxy)-2-
     hydroxy-3-isopropylaminopropane, m. 74-5°. DL-1-(2-Acetyl-4-
     nitrophenoxy) -2-hydroxy-3-isopropyl-aminopropane phenylsulfonylhydrazone-
     HCl m. 200-2°; DL-1-(2-acetyl-4-chlorophenoxy)-2-hydroxy-3-
     isopropylaminopropane phenylsulfonylhydrazone-HCl m. 208-9°;
     DL-1-(2-acetyl-4,6-dichlorophenoxy)-2-hydroxy-3-isopropylaminopropane
     2-naphthyl-sulfonylhydrazone-HCl m. 162-4°; DL-1-(2-acetyl-4,6-
     dichlorophenoxy) -2-hydroxy-3-isopropylaminopropane 1-naphthyl-
     sulfonylhydrazone-HCl m. 172°; DL-1-(2-acetyl-5-chlorophenoxy)-2-
     hydroxy-3-isopropylaminopropane phenylsulfonyl-hydrazone-HCl m.
     185-8°; II isonicotinoylhydrazone-HCl m. 21-2°. The
     tabulated VI were also prepared A mixture of 25 g. Me 3,5-dihydroxybenzoate,
     50 cc. 100% N2H4.H2O, and 100 cc. dry EtOH was refluxed for 5 hrs. to give
     3,5-dihydroxybenzhydra-zide, m. 265-6° (decomposition). Also were
     prepared 3,5-dichloro-4-methoxybenzhydrazide, m. 214-15°; and
    o-chlorophenylacetyl-hydrazide, m. 153-5.5°. DL-1-(4-Chloro-2-
    propionylphenoxy)-2-hydroxy-3-(1-methyl-3-phenylpropylamine) oxime-HCl
     hydrate m. 65° (decomposition). A mixture (48 g.) 1-(4-chloro-2-
    propionylphenoxy)-2,3-epoxypropane, 30 g. 3-amino-1-phenylbutane, and 150
    cc. anhydrous MeOH was refluxed 24 hrs. The MeOH was evaporated and the
residue
    heated at 120° for 12 hrs. and at 150° for 3 hrs. to give
    DL-1-(-4chloro-2-propionylphenoxy)-2-hydroxy-3-(1-methyl-3-
    phenylpropylamino)propane, m. 81-5°, phenylsulfonylhydrazone-HCl m.
     114-17°. II guanylhydrazone trinitrate m. 180-1°;
    DL-1-(o-acetylphenoxy)-3-cyclohexylamino-2-hydroxypropane
    phenylsulfonylhydrazone-HCl m. 194.5-97° (decomposition).
                                                                A mixture of 10
    g. 1-(o-acetylphenoxy)-2,3-epoxypropane, 10 cc. cyclohexylamine, and 35
    cc. anhydrous EtOH was refluxed 2 days to give DL-1-(o-acetylphenoxy)-3-
     cyclohexylamine-2-hydroxypropane, m. 88.5°. DL-1-(o-Acetylphenoxy)-
     3-benzylamino-2-hydroxypropane phenylsulfonyl-hydrazone-HCl m.
     175-8°. A mixture of 10 g. 1-(o-acetylphenoxy)-2,3-epoxypropane, 35
    cc. PhCH2NH2, and 35 cc. anhydrous MeOH was allowed to stand at room
temperature
    under N for 24 hrs. to give DL-1-(o-acetylphenoxy)-3-benzylamino-2-
    hydroxypropane-HCl, m. 140-4°. II semicarbazone-HCl m.
     188-90°; II phenylsulfonylhydrazone m. 161-2°; II
    p-chlorophenylsulfonyl-hydrazone m. 161-2°; II
    phenylsulfonylhydrazone di-p-toluoyl-tartrate m. 60° (decomposition). A
    mixture of 60 g. 1-(o-acetylphenoxy)-2,3-epoxypropane and 20 g.
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N-isopropylethylamine was refluxed until thin-layer chromatog. showed the reaction was complete, and dissolved in CHCl3. The solution was treated with excess dry HCl; the precipitate was treated with 2N NaOH and extracted with Et2O.

The extract was dried and treated with a solution of 17.3 g. di-p-toluoyltartaric acid in Et20 to give DL-1-(o-acetylphenoxy)-2-hydroxy-3-(N-isopropylmethylamino)propane di-p-toluoyltartrate. DL-1-(o-Acetylphenoxy)-2-hydroxy-3-(1-phenylethylamine)propane phenylsulfonylhydrazone m. 101-5° (decomposition). A mixture of 17.3 g. 1-(o-acetylphenoxy)-2,3-epoxypropane, 10.9 g. 1-phenylethylamine, and 150 cc. dry MeOH was refluxed for 36 hrs. to give DL-1-(o-acetylphenoxy)-2-hydroxy-3-(1-phenylethylamino)propane-HCl, m. 136-8°.

IT 22634-13-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 22634-13-5 HCAPLUS

CN p-Toluic acid, [o-[2-hydroxy-3-(isopropylamino)propoxy]-α-methylbenzylidene]hydrazide monohydrochloride, DL- (8CI) (CA INDEX NAME)

HC1

L58 ANSWER 37 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1969:77540 HCAPLUS

DN 70:77540

TI Antitubercular compounds. XLII. Preparation and antibacterial properties of certain derivatives of isomeric hydroxyphenylacetic acids

AU Lange, Jerzy; Urbanski, Tadeusz

CS Warsaw Polytech., Warsaw, Pol.

SO Dissertationes Pharmaceuticae et Pharmacologicae (1968), 20(6), 607-13

CODEN: DPHFAK; ISSN: 0012-3870

DT Journal

LA English

Amides, hydrazides, and hydroxamic acids of the 3 isomeric AB hydroxyphenylacetic acids are prepared Amides and hydrazides of m- and p-hydroxyphenylacetic acid were prepared by the routine method involving ammonolysis and hydrazinolysis of the corresponding esters. In the ortho-series this method yielded complex mixts. of unidentified products, whose separation and purification failed. Products of satisfactory purity were obtained, however, when o-hydroxyphenylaceto-lactone was used in place of the ester. The hydroxamic acids were synthesized by treating the corresponding esters with hydroxylamine in EtOH. The conversion of the Na salts into free acids by simple acidification was successful only with the para-isomer. The other 2 hydroxamic acids were prepared by precipitating Cu chelates and subsequently decomposing them with H2S. The following x-HOC6H4CH2COR were prepared (x, R and m.p. or b.p./mm. given): o, OMe, 71-2°; m, OEt, 177-9°/12; p, OEt, 187-9°/20; o, NH2, 113-14.5°; m, NH2, 122-3.5°; p, NH2, 174-5°; o, NHNH2, 154-5°; m, NHNH2, 169.5-71°; p, NHNH2,

199-200°; o, NHN:CHPh, 184-5°; m, NHN:CHPh, 189-90°; p, NHN:CHPh, 248-51°; o, NHOH, 95-6.5°; m, NHOH, 132.5-34°; p, NHOH, 176° (decomposition). The prepared compds. showed moderate or weak activity against several gram pos. and gram neg. bacteria strains.

22446-46-4P 22446-47-5P 22446-48-6P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

22446-46-4 HCAPLUS

CN Acetic acid, (o-hydroxyphenyl)-, benzylidenehydrazide (8CI) (CA INDEX NAME)

IT

RN

RN 22446-47-5 HCAPLUS

CN Acetic acid, (m-hydroxyphenyl)-, benzylidenehydrazide (8CI) (CA INDEX NAME)

RN 22446-48-6 HCAPLUS

CN Acetic acid, (p-hydroxyphenyl)-, benzylidenehydrazide (8CI) (CA INDEX NAME)

L58 ANSWER 38 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1967:55251 HCAPLUS

DN 66:55251

TI N-Substituted-phenyl fatty acid hydrazide derivatives

IN Kametani, Tetsuji

SO Jpn. Tokkyo Koho, 7 pp.

CODEN: JAXXAD

DT Patent

LA Japanese

FAN.CNT 1

PΙ

AB Manufacture of N-R1-2-R2-,4,5-R3-substituted phenylacetic hydrazide (I), useful as a potentiator for sedatives and for blood pressure depressants, was described. In an example, 0.5 g. 2-nitro-4,5-dimethoxyphenylacetic hydrazide is refluxed 5-10 min. in Me2CO to give 0.55 g. I (R1 =

isopropylidene, R2 = NO2, R3 = di-OMe), pale yellow, m. 178-9° (EtOH). Similarly prepared are the following I (R1, R2, R3, appearance, m.p., and % yield given): 3,4-dimethoxybenzylidene, NO2, di-OMe, pale yellow, 210-12° (C6H6), 80; benzylidene, Br, methylenedioxy, powder, 209° (EtOH), 90.9; 3,4-dimethoxybenzylidene, Br, methylenedioxy, powder, 204.5-6.5° (EtOH), 96.2; 3,4-methylenedioxybenzylidene, Br, methylenedioxy, powder, 212-13° (EtOH), 98.7; 3-methoxy-4-hydroxybenzylidene, Br, methylenedioxy, powder, 228° (EtOH), 93; 3-hydroxy-4-methoxybenzylidene, Br, methylenedioxy, powder, 204-6.5° (EtOH), 93; isopropylidene, Br, methylenedioxy, powder, 176-8° (EtOH), 69.8; α methylbenzylidene, Br, methylenedioxy, powder, 178-9° (EtOH), 82.4; propylidene, Br, di-OMe, microneedles, 153-4° (EtOH), 89.7; butylidene, Br, di-OMe, long needles, 138-9.5° (EtOH), 92.8; isobutylidene, Br, di-OMe, microneedles, 141-2° (EtOH), 84.4; crotonylidene, Br, di-OMe, pale yellow powder, 176-7° (EtOH), 73.8; 2-methylacrylidene, Br, di-OMe, pale yellow, 176-7° (EtOH), 79.5; benzylidene, Br, di-OMe, microneedles, 131.5-3.5° (EtOH), 74.7; hexylidene, Br, di-OMe, needles, 133-4° (EtOH), 77.9; heptylidene, Br, di-OMe, microneedles, 124.5-5° (EtOH), 82.5; octylidene, Br, di-OMe, microneedles, 126.5-7° (EtOH), 92.2; 2-ethylhexylidene, Br, di-OMe, columns, 126-7° (AcOEt), 85.6; nonylidene, Br, di-OMe, powder, 123-4° (EtOH), 86.1; decylidene, Br, di-OMe, powder, 125-6° (AcOEt), 77.1; undecylidene, Br, di-OMe, columns, 124.5-5.5° (EtOH), 83.9; cinnamylidene, Br, di-OMe, powder, 186-7° (C6H6), 86.0; β-phenylpropylidene, Br, di-OMe, pale orange flakes, 148.5-50.5° (EtOH), 80.3; 3,4-dimethoxybenzal, Br, di-OMe, needles, 209-9.5° (EtOH), 79.4; 3,4-methylenedioxybenzal, Br, di-OMe, needles, 228-8.5° (EtOH), 84.0; 3-methoxy-4hydroxybenzal, Br, di-OMe, short needles, 197-8° (EtOH), 87.6. Also is prepared 85% N-(3,4-dimethoxybenzylidene)-2-nitro-4,5dimethoxyphenylpropionic hydrazide, pale brown, m. 177-8° (EtOH). 14502-15-9P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 14502-15-9 HCAPLUS Acetic acid, (2-bromo-4,5-dimethoxyphenyl)-, benzylidenehydrazide (8CI)

(CA INDEX NAME)

TT

RN

CN

L58 ANSWER 39 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN AN1964:476235 HCAPLUS DN 61:76235 OREF 61:13218b-c TI Anticancer agents. IV. Desulfurization by hydrazine hydrate. 1. The reaction of 0-, m-, and p-nitrobenzyl disulfide with hydrazine hydrate ΑU Kametani, Tetsuji; Fukumoto, Keiichiro; Takayanagi, Yuriko; Teshigawar, Takashi; Umezawa, Osamu CS Tohoku Univ., Sendai, Japan so Chemical & Pharmaceutical Bulletin (1960), 8(11), 995-8 CODEN: CPBTAL; ISSN: 0009-2363 DTJournal LA Unavailable OS CASREACT 61:76235 AB cf. CA 54, 11018g; 61, 600d. When 0-, m-, or p-nitrobenzyl disulfide was refluxed with N2H4.H2O in EtOH, nitrobenzylidenehydrazines were formed, contrary to expectation, and reduction of the nitro group was not effected. Treatment of p-nitrobenzylidenehydrazine with HCl or H2SO4 gave bis(p-nitrobenzylidene)hydrazine, which formed an N-acetyl derivative by treatment with Ac2O.

RN 25996-47-8 HCAPLUS

CN Acetic acid, [(4-nitrophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

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L58 ANSWER 40 OF 40 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     1954:42359 HCAPLUS
DN
     48:42359
OREF 48:7580b-i,7581a
     Tuberculostatic hydrazides and their derivatives
TI
     Buu-Hoi, Ng. Ph.; Xuong, Ng. D.; Nam, Ng. H.; Binon, Fernand; Royer, Rene
AU
CS
     Univ. Paris
SO
     Journal of the Chemical Society, Abstracts (1953) 1358-64
     CODEN: JCSAAZ; ISSN: 0590-9791
DT
     Journal
     Unavailable
LA
AB
     cf. C.A. 47, 2358c. Hydrazides and their hydrazone condensation products
     with aldehydes and ketones (many derivs. selected for chelation ability)
     were prepared for determination of their tuberculostatic activities in vitro,
some
     of which are given. Hydrazides prepared were: salicylic (I), and its 5-Cl
     (II), m. 222°, 5-Br (III), m. 218°, 3,5-di-Cl (IV), m.
     175°, 3,5-di-Br (V), m. 192°, and 3,5-diiodo derivative (VI), m.
     218°; p-hydroxybenzoic (VII); 2-hydroxy-3-naphthoic (VIII);
     2-thiophenecarboxylic (IX), and its 5-Br (X), and 5-Cl derivative (XI);
     nicotinic (XII); iso-nicotinic (XIII); phenylacetic (XIV);
     2-naphthyloxyacetic (XV), m. 172°; phenoxyacetic (XVI), m.
     108°; dodecanoic (XVII); 2-hydroxy-1-naphthoic (XVIII), m.
     206° (decomposition); 1-, m. 169°, and 2-naphthylacetic, m.
     189°; 3,4-dichlorocinnamic, m. 138°. Hydrazones,
     RCONHN:CHR' [R', parent hydrazide (RCONHNH2), and m.p. given]: p-MeC6H4:
     X, 191°. o-ClC6H4: VIII, 263°; X, 208°; XI,
     210°; XII, 167°. p-ClC6H4: I, 262°; II, 276°;
     III, 275°; VIII, 266°; X, 225°; XII, 197°;
     XIV, 167°; XV, 215°; XVI, 175°; XVII, 102°.
     o-HOC6H4: I, 284°; II, 307°; III, 316°; VI,
     247°; VII, 280°; VIII, 301°; X, 239°; XI,
     229°; XII, 194°; XIII, 251°. m-HOC6H4: VII,
     271°. p-HOC6H4: II, 286°; III, 292°; VII,
     273°; X, 245°; XII, 248°; XV, 206°.
     p-MeOC6H4: II, 268°; III, 267°; VII, 226°; VIII,
     288°; X, 187°; XI, 175°; XIV, 171°; XV,
     182°; XVI, 138°. m-O2NC6H4: XI, 239°. p-Me2NC6H4:
     VII, 251°; VIII, 251°; X, 213°; XI, 207°;
     XIII, 199°; XVII, 103°. p-PhCH2OC6H3: VII, 232°.
     2,4-Cl2C6H3: VIII, 261°; IX, 231°; XI, 227°.
     3,4-Cl2C6H3: I, 256°; II, 264°; III, 274°; VIII,
     251°; X, 237°; XI, 244°; XII, 195°.
     3,4-(MeO)2C6H3: I, 197°; II, 239°; III, 241°; XII,
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158°; XV, 181°. 5,2-Cl(HO)C6H3: I, 287°; II,
310°; III, 313°; VIII, 240°; X, 233°; XI,
219°; XII, 206°; XIII, 232°; XVIII, 240°.
5,2-Br(HO)C6H3: X, 232°; XI, 222°. 2,3-HO(MeO)C6H3: I,
247°; II, 266°; III, 272°; VIII, 272°; X,
249°; XI, 245°; XIII, 234°. 4,3-HO(MeO)C6H3: XII,
218°. 3,4-MeO[Me(CH2)11]C6H3: VIII, 140°; IX, 112°;
XI, 141°; XII, 126°. 3,4-CH2O2C6H3: I, 271°; II,
263°; III, 253°; VII, 238°; VIII, 236°; XII,
209°; XIV, 219°; XV, 190°; XVI, 201°.
3,5,2-Cl2(HO)C6H2: I, 274°; II, 297°; III, 304°; IV,
286°; V, 238°; VI, 244°; VIII, 291°; X,
246°; XII, 215°; XIII, 244°. 3,5,2-Br2(HO)C6H2: I,
261°; II, 312°; III, 315°; IV, 290°; V,
266°; VI, 268°; VIII, 295°; XIII, 214°.
3,5-I2(HO)C6H2: I,258°; II, 319°; VI, 294°; IX,
261° (decomposition); X, 255°; XI, 264°; XIII,
213°. 3,5,4-I2(HO)C6H2: VII, 270°; XIII, 250°
(decomposition); PhCH:CH: VII, 232°; XIII, 201°.
Me2C:CH(CH2)2CMe:CH: VII, 140°. 1-Cl0H7: XII, 199°.
2,1-MeOC10H6: VIII, 223°. 5-Acenaphthenyl: VIII, 258°; X,
228°; XI, 231°; XII, 212°; XIII, 200°.
3-pyrenyl: VIII, 262°; X, 288°; XI, 288°; XII,
260°; XIII, 259°. 9-Ethyl-3-carbazolyl: XII, 220°;
XIII, 244°. Substituted isatin-3-hydrazones [substituent(s) on
isatin nucleus, parent hydrazide (RCONHNH2), and m.p.]: H (unsubstituted):
I, 326°; II, 311°; III, 315°; VIII, 332°; X,
242°; XII, 283°; XIII, 296°; XIV, 167°. 5-Br:
I, 318°; II, 313°; III, 312°; VIII, 320°; XII,
292°; XIII, 318°; XIV, 228°; XV, 252°; XVI,
201°; XVII, 166°. 5-Cl: II, 314°; III, 309°.
5-Me: I, 312°; II, 316°; III, 313°; VIII,
323°; XII, 266°; XIII, 316°; XV, 260°; XVIII,
130°. 7-Me: XII, 195°; XIII, 206°.
5-Substituted-2-thiophenecarboxaldehyde hydrazones: (substituent and m.p.)
Pr: II, 216°; III, 222°; X, 154°; XI, 153°.
Tetradecyl: XI, 107°. 2,4-Dichlorophenyl Me ketone hydrazones
(parenhydrazide and m.p. given): XII, 236°; XIII, 213°.
Glyoxal bis(p-hydroxybenzoylhydrazone) m. 300°. Hydrazones,
(CH2)n(CONHN:R')2, derived from adipic and sebacic hydrazides, resp.
(carbonyl compound and m.p. given): p-ClC6H4CHO, 248°, 209°;
p-MeOC6H4CHO, 217°, 182°; piperonal, 234°,
203°; p-Me2NC6H4CHO, 224°, 164°; 5-
acenaphthenecarboxaldehyde, 212°, 194°; isatin
(3,3'-compound), 232°, 192°; 5-bromoisatin, 233°,
242°; vanillin, 287°, -. Also prepared were: Et
3,4-dichlorocinnamate, m. 81°, and the 2,4-di-Cl isomer, m.
52°; dodecyl vanillyl ether, b18 256-8°, m. 57°
(thiosemicarbazone, m. 128°; semicarbazone, m. 142°;
4-oxo-2-thiazolinylhydrazone, m. 188°).
67759-87-9, Hydrazine, 1-p-chlorobenzylidene-2-phenylacetyl-
   (tuberculostatic activity of)
67759-87-9 HCAPLUS
Benzeneacetic acid, [(4-chlorophenyl)methylene]hydrazide (9CI) (CA INDEX
NAME)
```

IT

RN

CN

$$CH = N-NH-C-CH_2-Ph$$

=>



STIC Search Report Biotech-Chem Library

STIC Database Tracking Number

TO: Susan Hanley

Location: rem/3d70/3e71

Art Unit: 1651

Tuesday, April 26, 2005

Case Serial Number: 10/047251

From: Noble Jarrell

Location: Biotech-Chem Library

Rem 1B71

Phone: 272-2556

Noble.jarrell@uspto.gov

Search Notes		
	j.	
	•	
	· · · · · · · · · · · · · · · · · · ·	



10/047,251

Search Request:

- 1. Please do a structure search for each of the attached compounds with the modifications that I have specified. Where possible, I have indicated a structural feature common to all of the attached compounds so that you may be able to consolidate the compounds into the fewest searches possible.
- 2. Please see if the compounds from your search results have been used in the following methods:
- a. Does the compound inhibit any phosphatase?
- b. Does the compound decrease drug resistance in plants or mammals?
- c. Have the compounds ever been administered (i.e. sprayed, applied, etc.) to a plant such as peas, carrots, flowers, rice, wheat, any plant that you can think of.
- d. Have any of the compounds been used to inhibit (down-regulate, antagonist, etc) an ABC transporter (also known as an ABC-binding cassette) in a cell?

For the plants, the plant can be in a cell culture.

Thanks. Please call me if you have any questions 2-2508.

Susan

```
=> d his
```

(FILE 'HOME' ENTERED AT 08:10:27 ON 26 APR 2005)

FILE 'HCAPLUS' ENTERED AT 08:10:46 ON 26 APR 2005 L1 1 US20020173031/PN

FILE 'REGISTRY' ENTERED AT 08:11:24 ON 26 APR 2005

FILE 'HCAPLUS' ENTERED AT 08:11:25 ON 26 APR 2005 L2 TRA L1 1- RN : 23 TERMS

FILE 'REGISTRY' ENTERED AT 08:11:25 ON 26 APR 2005 L3 23 SEA L2

FILE 'WPIX' ENTERED AT 08:11:27 ON 26 APR 2005 L4 1 US20020173031/PN

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FILE COVERS 1907 - 26 Apr 2005 VOL 142 ISS 18 FILE LAST UPDATED: 25 Apr 2005 (20050425/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all 11

```
ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
     2000:628251 HCAPLUS
AN
DN
     133:219782
ED
     Entered STN: 10 Sep 2000
TI
     Genetic and epigenetic manipulation of ABC transporters and
     ecto-phosphatases for modulating drug resistance and methods for detection
     of ecto-phosphatase inhibitors
     Thomas, Collin E.; Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.;
IN
     Hurley, Laurence
     University of Texas, USA
     PCT Int. Appl., 85 pp.
SO
     CODEN: PIXXD2
DT
    Patent
     English
     ICM C12N005-04
IC
          C12N005-06; C12N001-16; C12N001-20; C12N015-67; C12N015-81;
     C12N015-82; C12N015-90; A01H001-00; A01H005-00
9-2 (Biochemical Methods)
     Section cross-reference(s): 1, 3, 10, 11
FAN. CNT 3
     PATENT NO.
                            KIND
                                   DATE
                                                 APPLICATION NO.
                                                                           DATE
                                   20000908
                                                                           20000228
PΙ
     WO 2000052144
                             A1
                                                 WO 2000-US5315
          W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
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KG,
                                        KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
                                                               RU,
                               MW,
                                        NO.
                                             NZ,
                                                          RO, RU, SD, SE, SG, SI, VN, YU, ZW, AM, AZ, BY,
              MD. MG.
                       MK.
                           MN,
                                    MX,
                                                 PL, PT,
              SK,
                           TM,
                               TR,
                                             UA, UG, UZ,
                  SL,
                       TJ,
                                    TT,
                                        TZ,
                      MD, RU, TJ,
              KG, KZ,
                                    TM
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          RW: GH, GM, KE, LS, MW,
                                    SD,
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                               GB, GR, IE, IT, LU, MC, NL, PT, GN, GW, ML, MR, NE, SN, TD, TG 20020313 EP 2000-913685
              DK,
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                  ES, FI,
                           FR,
                                                                   SE, BF, BJ, CF,
              CG, CI, CM,
                           GA,
     EP 1185623
                                                                          20000228
                            A1
                           DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              AT, BE, CH,
                  SI, LT, LV, FI, RO
              IE,
     US 2002173031
                                   20021121
                                                 US 2002-47251
                                                                          20020114 <---
                             A1
PRAI US 1999-261825
                                    19990303
                             A
     WO 2000-US5315
                                   20000228
CLASS
PATENT NO.
                          PATENT FAMILY CLASSIFICATION CODES
                  CLASS
 WO 2000052144
                   ICM
                           C12N005-04
                           C12N005-06; C12N001-16; C12N001-20; C12N015-67;
                   ICS
                           C12N015-81; C12N015-82; C12N015-90; A01H001-00;
                           A01H005-00
 US 2002173031
                  NCL
                           435/245.000; 435/195.000
                          A61K031/165+A; A61K031/166; A61K031/167; A61K031/18;
                  ECLA
                          A61K031/215L10; A61K031/216; A61K031/24; A61K031/352;
                           A61K031/381; A61K031/404; A61K031/425F; C07K014/705;
                           C12N009/14; C12N015/82C8B4
AB
     The present invention relates to methods for modulating the resistance of
     cells to foreign compds., i.e. drugs, antibiotics, etc. by altering the
     ATP gradient across biol. membranes. Altering the ATP gradient across
     biol. membranes is achieved through the manipulation of ecto-phosphatase activity and ABC transporter mol. activity. The above method may be
     useful to confer herbicide resistance to plants, antibiotic resistance to
     bacteria, and drug resistance to yeast cells, or to reduce resistance in
     cells, bacteria, and yeast in order to facilitate chemotherapeutic
     treatments. The present invention is also directed to the methods for
     identifying ecto-phosphatase inhibitors and uses thereof. Thus,
     Arabidopsis thaliana has been shown to possess an ecto-apyrase and this ecto-apyrase and PGP-1 (an MDR-like protein) to have a role in MDR.
     Addnl., the extracellular ATP pool was shown to be critical for MDR in yeast.
     Screening of a combinatorial library of small mols. has resulted in
     identification of apyrase inhibitors.
     drug resistance ectophosphatase ABC transporter ATP gradient
     Transport proteins
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
         (ABC; genetic and epigenetic manipulation of ABC transporters and
         ecto-phosphatases for modulating drug resistance and methods for
         detection of ecto-phosphatase inhibitors)
IT
     Membrane, biological
         (ATP gradient across; genetic and epigenetic manipulation of ABC
         transporters and ecto-phosphatases for modulating drug resistance and
         methods for detection of ecto-phosphatase inhibitors)
IT
     Chemotherapy
     Herbicide resistance
         (augmentation of; genetic and epigenetic manipulation of ABC
         transporters and ecto-phosphatases for modulating drug resistance and
         methods for detection of ecto-phosphatase inhibitors)
IT
     Neoplasm
         (decreasing drug resistance in; genetic and epigenetic manipulation of
         ABC transporters and ecto-phosphatases for modulating drug resistance
         and methods for detection of ecto-phosphatase inhibitors)
     Arabidopsis thaliana
     Aspergillus fumigatus
     Bacteria (Eubacteria)
     Drug resistance
     Lactococcus lactis
     Pea
     Plant cell
     Saccharomyces cerevisiae
     Yeast
         (genetic and epigenetic manipulation of ABC transporters and
```

```
ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
IT
      Animal cell
          (mammalian; genetic and epigenetic manipulation of ABC transporters and
          ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
      50-81-7, Ascorbic acid, uses 11098-84-3, Ammonium molybdate RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
IT
          (genetic and epigenetic manipulation of ABC transporters and
          ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
      9013-05-2, Phosphatase 41481-51-0
                                                    139963-64-7
                       171248-07-0
      168832-50-6
                                         291536-79-3
                                                          291536-80-6
                                                                           291536-81-7
      291536-82-8
                                                          291536-85-1
                       291536-83-9
                                         291536-84-0
                                                                           291536-86-2
                       291536-88-4
                                         291536-89-5
      291536-87-3
                                                          291536-90-8
                                                                           291536-91-9
      291536-92-0
      RL: BAC (Biological activity or effector, except adverse); BSU (Biological
      study, unclassified); BIOL (Biological study)
          (genetic and epigenetic manipulation of ABC transporters and
          ecto-phosphatases for modulating drug resistance and methods for
      detection of ecto-phosphatase inhibitors)
56-65-5, ATP, biological studies
RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
IT
      BIOL (Biological study); OCCU (Occurrence)
          (gradient of; genetic and epigenetic manipulation of ABC transporters
          and ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
RE. CNT 8
                 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Decottignies; J Biol Chem 1998, V273(20), P12612 HCAPLUS
(1) Decottignies; J Biol Chem 1998, V273(20), P12612 HCA

(2) Dudler; J Biol Chem 1992, V267(9), P5882 HCAPLUS

(3) Grant; Cancer Research 1994, V54, P357 HCAPLUS

(4) Kiba; Plant Cell Physiol 1995, V36(5), P809 HCAPLUS

(5) Lu; The Plant Cell 1998, V10, P267 HCAPLUS

(6) Sidler; The Plant Cell 1998, V10(10), P1632

(7) Thomas; Plant Physiol 1999, V119, P543 HCAPLUS

(8) Wang; J Biol Chem 1996, V271(17), P9898 HCAPLUS
=> b reg
FILE 'REGISTRY' ENTERED AT 08:12:06 ON 26 APR 2005
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                                25 APR 2005 HIGHEST RN 849177-50-0
DICTIONARY FILE UPDATES:
                                25 APR 2005 HIGHEST RN 849177-50-0
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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005
   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, * effective March 20, 2005. A new display format, IDERL, is now
* available and contains the CA role and document type information.
```

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more

Search done by Noble Jarrell

information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide 13 tot

ANSWER 1 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN

291536-92-0 REGISTRY

Entered STN: 28 Sep 2000 ED

Acetic acid, phenoxy-, 1-[(benzoylamino)methyl]-2-naphthalenyl ester (9CI) CN (CA INDEX NAME)

3D CONCORD

MF C26 H21 N 04

SR

CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL STN Files:

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE) 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 2 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN

ED

291536-91-9 REGISTRY
Entered STN: 28 Sep 2000
Benzamide, 3-[[(4-bromophenyl)amino]sulfonyl]-N-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

NGXT 1913 CN

FS 3D CONCORD

MF C19 H14 Br N3 05 S

STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

$$0.2N \qquad \qquad NH-C \qquad \qquad 0 \qquad NH-Br$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE) 8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 3 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN

291536-90-8 REGISTRY RN

ED

Entered STN: 28 Sep 2000 4-Thiazolidinone, 3-[[(4-methoxyphenyl)amino]methyl]-2-methylene-5-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

3D CONCORD

C19 H17 N3 O4 S MF

SR CA

STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 4 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN L3

RN

ED

291536-89-5 REGISTRY
Entered STN: 28 Sep 2000
Hexanoic acid, [(2-hydroxy-5-nitrophenyl)methylene]hydrazide (9CI) (CA CN INDEX NAME)

3D CONCORD FS

MF C13 H17 N3 O4

SR CA

STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

OH
$$N-NH-C-(CH_2)_4-Me$$
 NO_2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE) 7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 5 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN L3
- RN
- 291536-88-4 REGISTRY Entered STN: 28 Sep 2000 ED
- CN 2H-1-Benzopyran-3-carbothioic acid, 2-oxo-, S-heptyl ester (9CI) (CA INDEX NAME)
- 3D CONCORD FS
- C17 H20 O3 S MF
- SR CA
- CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE) 7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 6 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN

RN

ED

291536-87-3 REGISTRY
Entered STN: 28 Sep 2000
Acetic acid, (2, 4, 6-trimethylphenoxy)-, (phenylmethylene)hydrazide (9CI) CN (CA INDEX NAME)

3D CONCORD

MF C18 H20 N2 O2

SR CA

STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE) 7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 7 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN L3

RN

ED

291536-86-2 REGISTRY
Entered STN: 28 Sep 2000
Benzoic acid, 2-[[(4-chlorophenyl)amino]carbonyl]-, 2-propynyl ester (9CI) CN (CA INDEX NAME)

FS 3D CONCORD

MF C17 H12 C1 N 03

SR CA

STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE) 7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 8 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN

RN

- ED
- 291536-85-1 REGISTRY
 Entered STN: 28 Sep 2000
 Benzoic acid, 3-methyl-, [1-(2-naphthalenyl)ethylidene]hydrazide (9CI)

(CA INDEX NAME) 3D CONCORD

FS MF C20 H18 N2 O

SR CA

STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE) 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 9 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN L3

RN

291536-84-0 REGISTRY Entered STN: 28 Sep 2000

CN 1-Naphthaleneacetic acid, [(4-bromophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

OTHER NAMES:

NGXT 195 CN

FS 3D CONCORD

DR 328125-88-8

MF C19 H15 Br N2 O

SR CA

STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE) 8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 10 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN L3

RN

ED

291536-83-9 REGISTRY
Entered STN: 28 Sep 2000
Benzamide, N-(4a, 8a-dihydro-1-naphthalenyl)-3, 5-bis(1, 1-dimethylethyl)-CN (9CI) (CA INDEX NAME)

3D CONCORD FS

MF C25 H31 N O

SR CA STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE) 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 11 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN L3

291536-82-8 REGISTRY RN

ED Entered STN: 28 Sep 2000

1-Naphthaleneacetic acid, [(2-hydroxy-5-methylphenyl)methylene]hydrazide CN (9CI) (CA INDEX NAME)

3D CONCORD

MF C20 H18 N2 O2

SR

STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE) 7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 12 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN 291536-81-7 REGISTRY Entered STN: 28 Sep 2000 L3

RN

ED

Benzamide, 4-chloro-N-(3-chlorophenyl)-N-[(2,4-dichlorophenyl)methyl]-(9CI) (CA INDEX NAME) CN

MF C20 H13 C14 N O

SR

CA, CAPLUS, TOXCENTER, USPATFULL STN Files:

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE) 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 13 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN L3

291536-80-6 REGISTRY Entered STN: 28 Sep 2000

[1, 1'-Biphenyl]-4-sulfonamide, N-(3-methylphenyl)- (9CI) (CA INDEX NAME) OTHER NAMES:

CN

NGXT 191

3D CONCORD FS

MF C19 H17 N 02 S

SR CA

STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE) 8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 14 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN 291536-79-3 REGISTRY L3

RN

Entered STN: 28 Sep 2000 ED

Benzenamine, N-(3-hexyl-4-phenyl-2(3H)-thiazolylidene)-, monohydrobromide CN (9CI) (CA INDEX NAME)

MF C21 H24 N2 S . Br H

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

(352638-92-7) CRN

HBr

7 REFERENCES IN FILE CA (1907 TO DATE) 7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 15 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN L3
- RN
- 171248-07-0 REGISTRY Entered STN: 12 Dec 1995

Benzeneacetic acid, 1-oxo-2-phenyl-1H-inden-3-yl ester (9CI) (CA INDEX CN

NAME) 3D CONCORD FS

MF C23 H16 03

SR CA

CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL STN Files:

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE) 8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 16 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN

RN

168832-50-6 REGISTRY Entered STN: 13 Oct 1995 ED

Octanediamide, N, N'-bis(4-methylphenyl)- (9CI) (CA INDEX NAME) CN

FS 3D CONCORD

MF C22 H28 N2 O2

SR

STN Files: CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11 REFERENCES IN FILE CA (1907 TO DATE)

11 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 17 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN

RN

154201-55-5 REGISTRY Entered STN: 07 Apr 1994 ED

CN Benzo[b]thiophene-3-carboxylic acid, 2-[[(cyclohexylamino)acetyl]amino]-4, 5, 6, 7-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

3D CONCORD

MF C19 H28 N2 O3 S

CI COM

SR CA

STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE) 8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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ANSWER 18 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN 139963-64-7 REGISTRY Entered STN: 27 Mar 1992
L3
RN
```

ED

Ethanone, 2, 2'-thiobis[1-(1H-indol-3-yl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H16 N2 O2 S

SR CA

STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL LC (*File contains numerically searchable property data)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE) 8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 19 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN

41481-51-0 REGISTRY Entered STN: 16 Nov 1984 ED

Guanidine, N, N-dibutyl-N'-phenyl-N''-[(phenylamino)sulfonyl]- (9CI) (CA INDEX NAME)

C21 H30 N4 O2 S

LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL (*File contains numerically searchable property data)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE) 9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 20 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN L3

11098-84-3 REGISTRY Entered STN: 16 Nov 1984 ED

Ammonium molybdenum oxide (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Molybdic acid, ammonium salt

OTHER NAMES:

CN Ammonium molybdate

DR 12673-54-0, 11119-83-8, 11128-97-5

Unspecified MF

CI COM, MAN

IN Files: AGRICOLA, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMLIST, CIN, CSCHEM, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, TOXCENTER, STN Files: TULSA, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)

Other Sources: EINECS**, NDSL**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

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*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
               2002 REFERENCES IN FILE CA (1907 TO DATE)
                 61 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
               2004 REFERENCES IN FILE CAPLUS (1907 TO DATE)
      ANSWER 21 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN
L3
      9013-05-2 REGISTRY
RN
      Entered STN: 16 Nov 1984
Phosphatase (9CI) (CA INDEX NAME)
ED
OTHER NAMES:
CN
      4-Methylumbelliferyl phosphatase
CN
      Alkyl phosphomonoesterase
      Naphthol-AS-B1-phosphohydrolase
CN
CN
      Naphthol-AS-Bi-phosphohydrolase
CN
      Phosphoesterase
      Phosphohydrolase
CN
CN
      Phosphomonoesterase
CN
      Phosphoric acid esterase
DR
      9013-13-2
      Unspecified
MF
CI
      MAN
        IN Files: ADISNEWS, AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CBNB, CEN, CHEMLIST, CIN, CSCHEM, CSNB, EMBASE, IFICDB, IFIPAT, IFIUDB, MEDLINE, NAPRALERT, NIOSHTIC, PIRA, PROMT,
      STN Files:
         TOXCENTER, USPAT2, USPATFULL
      Other Sources:
                           EINECS**
            (**Enter CHEMLIST File for up-to-date regulatory information)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
             14279 REFERENCES IN FILE CA (1907 TO DATE)
64 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
14286 REFERENCES IN FILE CAPLUS (1907 TO DATE)
      ANSWER 22 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN \bf 56-65-5 REGISTRY
L3
     Entered STN: 16 Nov 1984
Adenosine 5'-(tetrahydrogen triphosphate) (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 5'-ATP
      Adenosine 5'-triphosphate
Adenosine 5'-triphosphoric acid
CN
CN
      Adenosine triphosphate
Adenosine, 5'-(tetrahydrogen triphosphate)
CN
CN
      Adenylpyrophosphoric acid
      Adephos
CN
CN
      Adetol
CN
      Adynol
CN
      Atipi
CN
      ATP
      ATP (nucleotide)
CN
CN
      Atriphos
CN
      Cardenosine
CN
      Fosfobion
CN
      Glucobasin
CN
      Myotriphos
CN
      Phosphobion
CN
      Striadyne
CN
      Triadenyl
CN
      Triphosphaden
CN
      Triphosphoric acid adenosine ester
```

10168-83-9, 16488-07-6, 51569-41-6, 71800-44-7, 84412-18-0 C10 H16 N5 013 P3

FS

DR MF CI STEREOSEARCH

STN Files:

COM

Search done by Noble Jarrell

ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*,

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BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DETHERM*, DRUGU, EMBASE, GMELIN*, IFICDB, IFIPAT, IFIUDB, IMSDRUGNEWS, IMSRESEARCH, IPA, MEDLINE, MRCK*, NAPRALERT, NIOSHTIC, PHAR, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, TULSA, USPAT2, USPATFULL (*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)
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Absolute stereochemistry.

CN

Cenetone

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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73409 REFERENCES IN FILE CA (1907 TO DATE)
1476 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
73465 REFERENCES IN FILE CAPLUS (1907 TO DATE)
19 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
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ANSWER 23 OF 23 REGISTRY COPYRIGHT 2005 ACS on STN 50-81-7 REGISTRY Entered STN: 16 Nov 1984
RN
     L-Ascorbic acid (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
      (+)-Ascorbic acid
CN
     3-keto-L-Gulofuranolactone
CN
     3-0xo-L-gulofuranolactone
CN
     Adenex
     Allercorb
     Antiscorbic vitamin
     Antiscorbutic vitamin
CN
     Ascoltin
CN
     Ascorbajen
CN
     Ascorbic acid
CN
     Ascorbicap
CN
     Ascorbutina
     Ascorin
     Ascorteal
CN
     Ascorvit
CN
     C-Quin
     Č-Vimin
CN
CN
     Cantan
CN
     Cantaxin
     Catavin C
CN
     Ce-Mi-Lin
CN
     Ce-Vi-Sol
CN
     Cebicure
CN
     Cebion
CN
     Cebion, Y-lactone
CN
     Cebione
CN
     Cecon
CN
     Cegiolan
     Ceglion
CN
     Ceklin
     Celaskon
CN
     Celin
CN
     Cell C
CN
     Cemagyl
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Cereon
CN
                  Cergona
                  Cescorbat.
                  Cetamid
                  Cetane
                  Cetane-Caps TC
CN
                  Cetebe
                  Cetemican
CN
                  Cevalin
                  Cevatine
                  Cevex
CN
                  Cevimin
CN
                  Cevital
CN
                  Cevitamic acid
                  Cevitamin
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for
                  DISPLAY
                  STEREOSEARCH
                  623158-95-2, 56533-05-2, 57304-74-2, 57606-40-3, 56172-55-5, 129940-97-2,
                  14536-17-5, 50976-75-5, 154170-90-8, 89924-69-6, 30208-61-8, 259133-78-3
CI
                  COM
                         IN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DIPPN*, DRUGUE, EMBASE, ENCOMPLIT, ENCOMPRISE, CHEMINE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DIPPN*, DRUGUE, EMBASE, ENCOMPLIT, ENCOMPRISE, CHEMINE, CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF THE CONTROL OF T
                  STN Files:
                          ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB,
                         IMSCOSEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PHAR, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USAN, USPAT2, USPATFULL, VETU, VTB
                                  (*File contains numerically searchable property data)
                  Other Sources: DSL**, EINECS**, TSCA**, WHO
                                  (**Enter CHEMLIST File for up-to-date regulatory information)
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Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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1595 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
73545 REFERENCES IN FILE CAPLUS (1907 TO DATE)
12 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> b wpix

FILE 'WPIX' ENTERED AT 08:12:17 ON 26 APR 2005 COPYRIGHT (C) 2005 THE THOMSON CORPORATION

FILE LAST UPDATED: 22 APR 2005 <20050422/UP>
MOST RECENT DERWENT UPDATE: 200526 <200526/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE, PLEASE VISIT:

http://www.stn-international.de/training_center/patents/stn_guide.pdf <<<

>>> FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE http://thomsonderwent.com/coverage/latestupdates/

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>>> FOR INFORMATION ON ALL DERWENT WORLD PATENTS INDEX USER
    GUIDES, PLEASE VISIT: http://thomsonderwent.com/support/userguides/
                                                                        (((
>>> NEW! FAST-ALERTING ACCESS TO NEWLY-PUBLISHED PATENT
    DOCUMENTATION NOW AVAILABLE IN DERWENT WORLD PATENTS INDEX
    FIRST VIEW - FILE WPIFV.
    FOR FURTHER DETAILS: http://www.thomsonderwent.com/dwpifv <<<
>>> THE CPI AND EPI MANUAL CODES HAVE BEEN REVISED FROM UPDATE 200501.
    PLEASE CHECK:
http://thomsonderwent.com/support/dwpiref/reftools/classification/code-revision/
    FOR DETAILS. <<<
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L4
     2003-456227 [43]
CR
                           DNC C2000-175136
DNN N2000-434619
     Increasing or decreasing drug resistance in target bacteria, yeast, plant
     or mammalian cells comprises altering ATP gradient across biological
     membrane of target cell.
DC
     B04 C06 P13
     HURLEY, L; LLOYD, A M; ROUX, S J; THOMAS, C E; WINDSOR, J B
IN
     (TEXA) UNIV TEXAS; (TEXA) UNIV TEXAS SYSTEM
PA
CYC
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     WO 2000052144
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             FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL
             TJ TM TR TT TZ UA UG UZ VN YU ZW
     AU 2000035084 A 20000921 (200065) C12N005-04
EP 1185623 A1 20020313 (200225) EN C12N005-04
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     US 2002173031
                       A1 20021121 (200279)
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     WO 2000052144 A1 WO 2000-US5315 20000228; AU 2000035084 A AU 2000-35084
     20000228; EP 1185623 A1 EP 2000-913685 20000228, WO 2000-US5315 20000228; US 2002173031 A1 Div ex US 1999-261825 19990303, US 2002-47251 20020114
     AU 2000035084 A Based on WO 2000052144; EP 1185623 A1 Based on WO
      2000052144
PRAI US 1999-261825
                             19990303; US 2002-47251
     ICM C12N001-36; C12N005-04
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AB
     WO 200052144 A UPAB: 20041104
     NOVELTY - Increasing or decreasing drug resistance in target bacteria,
     yeast, plant or mammalian cells comprises altering the ATP gradient across
     the biological membrane of the target cell.
           DETAILED DESCRIPTION - INDEPENDENT CLAIMS are included for:
           (i) altering the ATP gradient across the biological membrane of a
     target bacteria, yeast, plant or mammalian cell to achieve an increase in
     drug resistance comprising up-regulating an ecto-phosphatase in the target
           (ii) altering the ATP gradient across the biological membrane of a
      target bacteria, yeast, plant or mammalian cell to achieve an decrease in
     drug resistance comprising down-regulating an ecto-phosphatase in the
     target cell;
           (iii) altering the ATP gradient across the biological membrane of a
     plant cell to achieve an increase in drug resistance comprising
     up-regulating an ABC transporter in the target cell;
           (iv) altering the ATP gradient across the biological membrane of a
     plant cell to achieve an decrease in drug resistance comprising
     down-regulating an ABC transporter in the target cell;
           (v) augmenting the chemotheraputic effectiveness of a chemotheraputic
     molecule by decreasing resistance to the chemotheraputic molecule in a
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target cell comprising down-regulating an ecto-phosphatase in the target

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cell;
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(vi) conferring herbicide resistance to a plant comprising

up-regulating an ecto-phosphatase in the target cell;

(vii) increasing sensitivity to a drug molecule to inhibit or ameliorate micro-organism infection by altering the ATP gradient across the biological membrane of the micro-organism to achieve a decrease in drug resistance comprising down-regulating an ecto-phosphatase in the target cell;

(viii) inhibiting an ecto-phosphatase comprising administration of a compound selected from (3-hexyl-4-phenyl-3H-thiazol-2-ylidene)-phenyl-amine hydrobromide (I), biphenyl-4-sulfonic acid m-tolylamide (II), N,N-di-n-butyl-N'-phenyl-N''-phenylaminosulfonylguanidine (III), 4-chloro-N-(3-chloro-phenyl)-N-(2,4-dichloro-benzyl)-benzamide (IV), 1-(1H-indol-3-yl)-2-(2-(1H-indol-3-yl)-2-oxo-ethylsulfanyl)-ethanone (V), naphthalen-1-yl-acetic acid (2-hydroxy-5-methyl-benzylidene)-hydrazide (VI), 3,5-di-tert-butyl-N-naphthalen-l-yl-benzamide (VII), naphthalen-1-yl-acetic acid (4-bromo-benzylidene)-hydrazide (VIII), phenyl-acetic acid 3-oxo-2-phenyl-3H-inden-1-yl ester (IX), 3-methyl-benzoic acid (1-naphthalen-2-yl-ethylidene)-hydrazide (X), octanedioic acid bis-p-tolylamide (XI), N-(4-chloro-phenyl)-phthalamic acid prop-2-ynyl ester (XII), (2,4,6-trimethyl-phenoxy)-acetic acid benzylidene-hydrazide (XIII), 2-oxo-2H-chromene-3-carbothioic acid S-heptyl ester (XIV), hexanoic acid (2-(2-hydroxy-5nitrophenyl)ethylidene) hydrazide (XV), 2-(2-cyclohexylamino-acetylamino)-4, 5, 6, 7-tetrahydro-benzo(b) thiophene-3-carboxylic acid ethyl ester (XVI), 3-((4-methoxy-phenylamino)-methyl)-2-methylene-5-(4-nitro-benzylidene)thiazolidin-4-one (XVII), 3-(4-bromo-phenylsulfamoyl)-N-(3-nitro-phenyl)benzamide (XVIII) and phenoxy-acetic acid 1-(benzoylamino-methyl)-naphthalen-2-yl ester (XIX); and

(ix) decreasing drug resistance in target bacteria, yeast, plant or mammalian cells comprising administration of (I)-(XIX).

ACTIVITY - Antibacterial; fungicide.

MECHANISM OF ACTION - Ecto-phosphatase inhibitor.

USE - The method is useful for modulating drug resistance of cells. It is useful for increasing the sensitivity of cells to chemotheraputic and antibiotic agents and increasing resistance to herbicides. Dwg. 0/11

CPI GMPI FS

FA AB; DCN

CPI: B06-A01; B06-B01; B06-D01; B07-F01; B10-A08; B10-A19; B10-D03; B10-F02; B14-A01; B14-A04; B14-D07A; B14-M01E; B14-M01F; C06-A01; C06-B01; C06-D01; C07-F01; C10-A08; C10-A19; C10-D03; C10-F02; C14-A01; C14-A04; C14-A06; C14-D07A; C14-M01E; C14-M01F

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L11
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L12
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SAV TEM HAN251F0/A L13
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L17
                STR L11
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                D SCA
                D QUE STA L18
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STR L22

D SCA L16

D STR TOT

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L62
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                  E E3+ALL
                  E E3+ALL
           22680 SEA ABB=ON PLU=ON PLANT TISSUE CULTURE+OLD, NT/CT
L64
                  E ABC/CT
                  E E5+ALL
                  E TRANSPORT PROTEINS/CT
                  E E3+ALL
L65
            2858 SEA ABB=ON PLU=ON TRANSPORT PROTEINS+OLD, NT/CT (L) (ABC OR
                ATP (1A) BIND? (1A) CASSETT?)

O SEA ABB=ON PLU=ON L51 AND (L59 OR L60 OR L61 OR L62 OR L63
L66
                  OR L64 OR L65)
=> b reg
FILE 'REGISTRY' ENTERED AT 10:16:38 ON 26 APR 2005
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```

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 APR 2005 HIGHEST RN 849177-50-0 DICTIONARY FILE UPDATES: 25 APR 2005 HIGHEST RN 849177-50-0

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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

```
=> d que sta 116
L11 STR
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VAR G1=11/21 VAR G2=0/S NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 1 15 21 NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE

6458 SEA FILE=REGISTRY SSS FUL L11 L13 L14

VAR G3=1/2/3 VAR G4=H/AK VAR G5=16/17/18 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 15 4 NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

5 SEA FILE=REGISTRY SUB=L13 CSS FUL L14

5 ANSWERS 100.0% PROCESSED 6448 ITERATIONS (2 INCOMPLETE)

SEARCH TIME: 00.00.01

=> d que sta 121

VAR G1=11/21 VAR G2=0/S NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 1 15 21 NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE

6458 SEA FILE=REGISTRY SSS FUL L11 L13 L17 STR

VAR G2=0/S VAR G3=1/2/3VAR G4=H/X NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 21 4 NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L19

10 SEA FILE=REGISTRY SUB=L13 SSS FUL L17
5 SEA FILE=REGISTRY ABB=ON PLU=ON (291536-86-2/BI OR 339059-04-0/BI OR 412957-70-1/BI OR 412964-90-0/BI OR 412964-91-1/BI) L21

AND L19

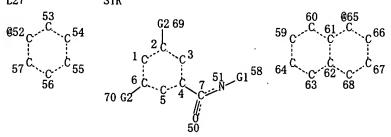
=> d que sta 133 L22 STR

VAR G1=58/60 VAR G2=37/52 VAR G3=0/S NODE ATTRIBUTES: CONNECT IS E2 RC AT 58 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 4 68 62 NUMBER OF NODES IS 49

STEREO ATTRIBUTES: NONE

2913029 SEA FILE=REGISTRY ABB=ON PLU=ON NR>=2 AND O>=1 AND N=1 32835 SEA FILE=REGISTRY SUB=L24 SSS FUL L22 L24 L26 L27



VAR G1=52/65 VAR G2=H/AK NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 52 4 59 NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

55 SEA FILE=REGISTRY SUB=L26 CSS FUL L27 L29 L30

43 SEA FILE=REGISTRY ABB=ON PLU=ON L29 NOT (PMS/CI OR D/ELS)
QUE ABB=ON PLU=ON (PMS OR MAN OR IDS)/CI OR COMPD OR C L31

OMPOUND OR UNSPECIFIED OR (D OR T)/ELS 30 SEA FILE-REGISTRY ABB-ON PLU-ON L30 NOT L31 L32

```
=> d aue sta 136
'AUE' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'STA' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
```

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

- Index Name, MF, and structure - no RN SAM - All substance data, except sequence data - FIDE, but only 50 names IDE

SQIDE - IDE, plus sequence data

SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used

SQD - Protein sequence data, includes RN

SQD3 - Same as SQD, but 3-letter amino acid codes are used SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

APPS -- Application and Priority Information

BIB -- CA Accession Number, plus Bibliographic Data

CAN - CA Accession Number

CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

IND - Index Data

IPC - International Patent Classification

PATS — PI, SO STD — BIB, IPC, and NCL

IABS — ABS, indented, with text labels IBIB — BIB, indented, with text labels

ISTD - STD format, indented

OBIB ----- AN, plus Bibliographic Data (original) OIBIB ----- OBIB, indented with text labels

SBIB ---- BIB, no citations SIBIB ---- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS — To see a complete list of individual display fields. HELP FORMATS — To see detailed descriptions of the predefined formats. ENTER DISPLAY FORMAT (IDE): end

=> d que sta 136 L34

VAR G1=63/64/65 VAR G2=70/71/72 VAR G3=H/X VAR G4=1/2/3 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 68 62 4 NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

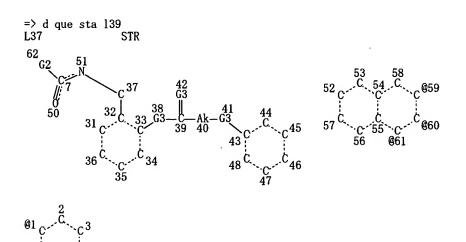
L36

24 SEA FILE=REGISTRY SSS FUL L34

100.0% PROCESSED 9855 ITERATIONS

24 ANSWERS

SEARCH TIME: 00.00.01



VAR G2=1/58/59/60/61 VAR G3=0/S NODE ATTRIBUTES: CONNECT IS E2 RC AT 37 CONNECT IS E2 RC AT 51 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

```
GRAPH ATTRIBUTES:
RSPEC 52 4
NUMBER OF NODES IS 38
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STEREO ATTRIBUTES: NONE

L39 8 SEA FILE=REGISTRY SSS FUL L37

100.0% PROCESSED 2807 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.01

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FILE COVERS 1907 - 26 Apr 2005 VOL 142 ISS 18 FILE LAST UPDATED: 25 Apr 2005 (20050425/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all fhitstr 150 tot

```
L50 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
     2005:141200 HCAPLUS
     142:254568
DN
ED
     Entered STN: 18 Feb 2005
ΤI
     Methods and compositions for increasing the efficacy of
     biologically-active ingredients such as antitumor agents
     Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.; Thomas, Collin E.
IN
     Board of Regents, the University of Texas System, USA PCT Int. Appl., 243 pp.
S0
     CODEN: PIXXD2
DT
     Patent
     English
LA
     ICM C12N
IC
     1-6 (Pharmacology)
FAN. CNT 1
```

	PATENT NO.					D	DATE		APPLICATION NO.					DATE			
ΡI	WO 2005014777				A2		20050217		WO 2003-US32667					20031016			
	P	7: AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		C0,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	GE,
		GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,
		LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,
		OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,
		TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW		
	F	RW: GH,					MZ,									AZ,	BY,
		KG,	KZ,				TM,										
		FI,					IE,										
		BF.					CM,										
PRAI	PRAI US 2002-418803P						2002		•	٠,	•	_,		•	•	•	

CLASS PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES WO 2005014777 ICM C12N The invention provides methods and compns. for modulating the sensitivity of cells to cytotoxic compds. and other active agents. In accordance with the invention, compns. are provided comprising combinations of ectophosphatase inhibitors and active agents. Active agents include antibiotics, fungicides, herbicides, insecticides, chemotherapeutic agents, and plant growth regulators. By increasing the efficacy of active agents, the invention allows use of compns. with lowered concns. of active ingredients. ST antibiotic fungicide herbicide insecticide plant growth regulator combination antitumor IT Trichoderma polysporum ((ATCC 20475; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Trichoderma harzianum ((ATCC 20476); methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Pseudomonas fluorescens (1629RS; methods and compns. for increasing the efficacy of biol. -active ingredients such as antitumor agents) IT Pseudomonas fluorescens (A506; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Zeolites (synthetic), biological studies Zeolites (synthetic), biological studies Zeolites (synthetic), biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (Ag; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) IT Surfactants (Alkanolamide; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (Bacillus thuringiensis CrylF and CfylAb; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents) Balsams IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (Canadian; methods and compns. for increasing the efficacy of biol. -active ingredients such as antitumor agents) Alcohols, biological studies Alcohols, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (C11-15-secondary, ethoxylated; methods and compns. for increasing the efficacy of biol. -active ingredients such as antitumor agents) Isoalkanes RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(C12-14; methods and compns. for increasing the efficacy of

biol.-active ingredients such as antitumor agents)

Alcohols, biological studies

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(C12-15; methods and compns. for increasing the efficacy of biol. -active ingredients such as antitumor agents)

Alcohols, biological studies

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(C6-12; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)

IT Diglycerides

Glycerides, biological studies

```
Monoglycerides
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (C8-10 monoglycerides and diglycerides; methods and compns. for
        increasing the efficacy of biol.-active ingredients such as antitumor
        agents)
     Alcohols, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
IT
     (Biological study); USES (Uses)
        (C8-10; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Pseudomonas fluorescens
        (EG-1053; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Bacillus subtilis
        (GBO3; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Pheromones, animal
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (German cockroach; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Fats and Glyceridic oils, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (Japan wax; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Sarcoma
        (Kaposi's; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Paraffin oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (Low mol. weight; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Bacillus subtilis
        (MBI 600; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Gene, animal
     RL: BSU (Biological study, unclassified); BIOL (Biological study) (MDR, Arabidopsis thaliana; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IΤ
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (Melaleuca alternifolia; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Balsams
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (Peru; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Bacillus subtilis
         (QST 713 strain; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Named reagents and solutions
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (Stoddard; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Paecilomyces lilacinus
         (Strain 251; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Lymphoproliferative disorders
IT
        (Waldenstrom's macroglobulinemia; methods and compns. for increasing
        the efficacy of biol. -active ingredients such as antitumor agents)
IT
     Kidney, neoplasm
        (Wilms'; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Leukemia
```

```
(acute lymphocytic; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
    Urethanes
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (adhesives; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Immunostimulants
        (adjuvants; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Silica gel, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (aerogel; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Flours and Meals
        (alfalfa; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Amines, biological studies
     Amines, biological studies
     Petroleum resins
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (aliphatic; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Delphinium
        (alkaloid; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
    Helleborus
     Schoenocaulon
        (alkaloids; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Quaternary ammonium compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (alkylbenzyldimethyl, chlorides; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
     Quaternary ammonium compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
(alkyltrimethyl, bromides; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
    Quaternary ammonium compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (alkyltrimethyl, chlorides; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
     Glycosides
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (amino; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (anise; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
    Antitumor agents
        (antibiotic; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Cytotoxic agents
        (antimetabolites; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
    Antibiotics
     Drug resistance
        (antitumor; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
    Paecilomyces fumoso-roseus
        (apopka strain 97; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
```

```
IT
     Petroleum, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (aromatic, alkylated; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
         (barley; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Quaternary ammonium compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (benzyl(hydrogenated tallow alkyl)dimethyl, salts with bentonite;
        methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Quaternary ammonium compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (benzyl-C12-14-alkyldimethyl; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
ΙT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (bergamot; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Prunus amygdalus
         (bitter almond; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Slags
IT
         (blast-furnace; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Linseed oil
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (boiled; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (cade; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (cajuput; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Caseins, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
ΙT
         (calcium complexes; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (camphor; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Gelatins, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (capsules; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Head, neoplasm
         (carcinoma; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Milk substitutes
         (cattle; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (cedar leaf; methods and compns. for increasing the efficacy of
```

```
biol. -active ingredients such as antitumor agents)
IT
     Essential oils
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (cedarwood; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Uterus, neoplasm
        (cervix; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (chamomile; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
ΙT
    Perfumes
        (cherry fragrance oil 493; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
     Paraffin waxes, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (chloro; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Carcinoma
     Chorion, neoplasm
        (choriocarcinoma; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Leukemia
        (chronic lymphocytic; methods and compns. for increasing the efficacy
        of biol. -active ingredients such as antitumor agents)
IT
    Leukemia
        (chronic myelocytic; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
    Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (cinnamon; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Essential oils
IΤ
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (citronella; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Cellulose pulp
        (citrus; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (citrus; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Essential oils
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (clove; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
ĪΤ
    Naphtha
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (coal; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
    Amines, biological studies
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (coco alkyl, compds. with tetrachlorophenol (1:1); methods and compns.
        for increasing the efficacy of biol.-active ingredients such as
        antitumor agents)
    Amides, biological studies
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
IT
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(coco, N-(hydroxyethyl); methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
    Fatty acids, biological studies
     Fatty acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (coco, cadmium salts; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
IT
     Intestine, neoplasm
        (colon; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
    Bentonite, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (compound with dimethyldioctadecylammonium chlorid; methods and compns.
        for increasing the efficacy of biol. -active ingredients such as
        antitumor agents)
    Naphthenic acids, biological studies
Naphthenic acids, biological studies
     Resin acids
     Resin acids
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (copper salts; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Food analysis
        (corn-containing, hydrolyzed; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
IT
     Flours and Meals
        (corn; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
ΙT
     Flours and Meals
        (cottonseed; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Avena sativa
     Triticum aestivum
        (cracked; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
        (crumb; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Syzygium aromaticum
        (crushed; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Isoalkanes
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (c11-12; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Quaternary ammonium compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (dicoco alkyldimethyl, chlorides; methods and compns. for increasing
        the efficacy of biol. -active ingredients such as antitumor agents)
     Fatty acids, biological studies
ĪΤ
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (dimer acids; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IΤ
     Urogenital tract
        (disease; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Coal tar
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (distillate, heavy oils; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
IT
     Coal tar
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
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(distillate, upper; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Petroleum products
        (distillates, C12-30-aromatic; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
ΙT
     Petroleum products
        (distillates, aliphatic; methods and compns. for increasing the efficacy
        of biol. -active ingredients such as antitumor agents)
     Petroleum products
IT
         (distillates, aromatic; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
ΙT
        (distillates, refined; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
ΙT
     Petroleum products
        (distillates; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Lime (chemical)
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (dolomitic; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Blood
        (dried; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
ΙT
     High throughput screening
        (drug; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Nicotiana tabacum
        (dust; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Uterus, neoplasm
        (endometrium, adenocarcinoma; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
IT
     Linseed oil
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (epoxidized; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Myeloproliferative disorders
        (essential thrombocythemia; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
ΙT
    Fatty acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (esters; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Monoglycerides
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (ethoxylated coco; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
    Lanolin
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (ethoxylated, acetate; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
IT
    Lanolin
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (ethoxylated; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (eucalyptus; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Allium cepa
     Glycine max
     Juniperus communis
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Malt
     Myrica cerifera
         (extract; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Lonchocarpus
        (exts.; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Alcohols, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (fatty; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
    Fats and Glyceridic oils, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (fish; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Cottonseed
     Glycine max
     Secale cereale
     Zea mays
        (flour and meal; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Juglans regia
     Wood
        (flour; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
    Polyesters, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (foam, UL-94 HF1 listed; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
        (fungoides; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Repellents
        (game; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Disease, animal
        (genitourinary; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (geranium; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
    Vitis vinifera
         (grape pomace; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Pseudotsuga menziesii
        (ground bark; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
ΙT
     Zea mays
        (ground cobs; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Oryza sativa
        (ground hulls; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Sesamum indicum
        (ground plant; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Avena sativa
        (ground; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
ΙT
        (hairy-cell; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Wood
        (hard, oil; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
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IT
     Carcinoma
        (head; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Naphtha
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (heavy aromatic; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Petroleum, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (heavy paraffinic distillate; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Drug screening
        (high throughput; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Coal tar pitch
        (high-temperature; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Glycine max
        (hulls; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
    Neoplasm
        (humoral hypercalcemia of malignancy; methods and compns. for
        increasing the efficacy of biol.-active ingredients such as antitumor
        agents)
ΙT
    Resin acids
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (hydrogenated, Me esters; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
ΙT
     Castor oil
     Soybean oil
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (hydrogenated; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Syrups (sweetening agents)
IT
        (hydrolyzed starch; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Paraffin waxes, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (hydrotreated; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Pancreatic islet of Langerhans, neoplasm
        (insulinoma; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Syrups (sweetening agents)
        (invert; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Antibacterial agents
        (iodophors; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
ΙT
    Pigments, nonbiological
         (iron oxide; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Bacillus subtilis
        (isolate B246; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Ampelomyces quisqualis
        (isolate M-10; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Essential oils
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (jasmine; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
    Paints
        (latex; methods and compns. for increasing the efficacy of biol.-active
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ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (lavender; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Naphthenic acids, biological studies
IT
     Naphthenic acids, biological studies
     Naphthenic acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (lead salts; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Eucalyptus
     Mentha pulegium
        (leaves; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
ΙŦ
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (lemon; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (lemongrass; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Skin, disease
        (lesion; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (lime; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Capsicum annuum annuum
        (longum group, paprika; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
IT
     Beta vulgaris saccharifera
     Fish
     Meat
     Medicago sativa
         (meal; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Flours and Meals
        (meat meal; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Fats and Glyceridic oils, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (menhaden; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Naphthenic acids, biological studies
     Naphthenic acids, biological studies
Naphthenic acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (mercury salts; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Acacia
     Adrenal cortex, neoplasm
     Agrobacterium tumefaciens
     Agrobacterium vitis
     Agrotis segetum granulovirus
     Alkylating agents, biological
     Allium cepa
     Allium sativum
     Ampelomyces quisqualis
     Anthracene oil
     Antibiotic resistance
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Arabidopsis thaliana Arachis hypogaea Aschersonia aleyrodis Avena sativa Bacillus sphaericus Bacillus thuringiensis Beeswax Bladder, neoplasm Bone meal Brain, neoplasm Bran Capsicum Caramel (color) Carcinoid Chamomile Cheese Cinnamon (horticultural common name) Combination chemotherapy Cork Corncob Cottonseed meal Creosote Cytotoxic agents Daucus carota Desmodium Drug delivery systems Drug screening Drugs Esophagus, neoplasm Fumigants **Fungicides** Gentiana Glues Glues Gossypium hirsutum Herbicides Hodgkin's disease Honey Human Insecticides Jet aircraft fuel Liliopsida Lung, neoplasm Magnoliopsida Mammary gland, neoplasm Meat Medicago sativa Melanoma Mentha piperita Milk Mint Molasses Multiple myeloma Nicotiana tabacum Nucleopolyhedrovirus Oatmeal Odor and Odorous substances Oryza sativa Ovary, neoplasm Paenibacillus popilliae **Paints** Paper Paperboard Peanut butter Phlebia gigantea Phlebiopsis gigantea Polycythemia vera Prostate gland, neoplasm Pseudomonas chlororaphis

Puccinia canaliculata

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Quassia
Quillaja
Rabbit calicivirus
Raisin
Repellents
Rosmarinus officinalis
Sawdust
Seaweed
Sinorhizobium meliloti
Skin, neoplasm
Solanum tuberosum
Solvent naphtha
Solvent naphtha
Solvent naphtha
Solvent naphtha
Sorghum bicolor
Sphagnum
Staphylococcus aureus
Stomach, neoplasm
Testis, neoplasm
Theobroma cacao
Theobroma cacao
Thickening agents
Thymus (plant)
Tomato mosaic virus
Trigonella foenum-graecum
Triticum aestivum
Verticillium lecanii
Wheat flour
Wheat flour
Whey
Wool
Yeast
Zea mays
   (methods and compns. for increasing the efficacy of biol.-active
   ingredients such as antitumor agents)
Amino acids, biological studies
Androgens
Asbestos
Asphalt
Bentonite, biological studies
Canola oil
Carbon black, biological studies
Caseins, biological studies
Castor oil
Chlorinated natural rubber
Coal tar
Coal tar
Coal tar
Coconut oil
Cod liver oil
Collagens, biological studies
Corn oil
Corticosteroids, biological studies
Cottonseed oil
Creosote oil
Cytokinins
Diatomite
Epoxy resins, biological studies
Essential oils
Feldspar-group minerals
Fertilizers
Gasoline
Gelatins, biological studies
Gibberellins
Glycopeptides
Granite, biological studies
Growth regulators, plant
Humic acids
Hydrocarbon oils
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Hydrocarbon oils
Jojoba oil
Kaolin, biological studies
Kerosene
Lard
Ligroine
Lime (chemical)
Linseed oil
Macrolides
Mica-group minerals, biological studies
Naphthenic acids, biological studies
Naphthenic oils
Natural products, pharmaceutical
Nitrile rubber, biological studies
Olive oil
Palm oil
Paraffin oils
Paraffin oils
Paraffin waxes, biological studies
Peanut oil
Perlite
Petrolatum
Petroleum hydrocarbons
Petroleum resins
Petroleum spirits
Phenols, biological studies
Phosphoproteins
Plastics, biological studies
Polyamides, biological studies
Polyamides, biological studies
Polyamines
Polyenes
Polyoxyalkylenes, biological studies
Polysiloxanes, biological studies
Polysiloxanes, biological studies
Polysiloxanes, biological studies
Polyurethanes, biological studies
Polyvinyl butyrals
Progestogens
Protein hydrolyzates
Pumice
Pyrethrins
Pyrethrins
Pyrethrins
Pyrethrins
Rape oil
Resins
Rosin
Rubber, biological studies
Safflower oil
Sand
Saponins
Shale
Shellac
Silica gel, biological studies
Soaps
Soapstone
Soybean oil
Tall oil
Tallow
Tetracyclines
Tung oil
Turpentine
Waxes
Wood tar
Zeins
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
   (methods and compns. for increasing the efficacy of biol.-active
   ingredients such as antitumor agents)
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Fats and Glyceridic oils, biological studies
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (mink; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
ΙT
    Anagrapha falcifera
        (multi-nuclear polyhedrosis virus (AFMNPV); methods and compns. for
        increasing the efficacy of biol.-active ingredients such as antitumor
        agents)
IT
    Skin, neoplasm
        (mycosis fungoides; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
ΙT
        (neck; methods and compns. for increasing the efficacy of biol. -active
        ingredients such as antitumor agents)
IT
    Abies
        (needle oil; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Neck, anatomical
        (neoplasm, carcinoma; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
    Nerve, neoplasm
        (neuroblastoma; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Chloramines
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (nitrogen mustards; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Fuel oil
        (number 1; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
    Diesel fuel
     Fuel oil
        (number 2; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
    Fuel oil
        (number 4; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
ΙT
    Fuel oil
        (number 6; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
    Lymphoma
        (non-Hodgkin's; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Surfactants
        (nonionic; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Alkanes, biological studies
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (normal C5-20; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Neodiprion sertifer
        (nuclear polyhedrosis virus; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
ΙT
    Aloe barbadensis
     Lavandula hybrida
        (oil; methods and compns. for increasing the efficacy of biol. -active
        ingredients such as antitumor agents)
    Resins
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
(oleoresins, capsicum; methods and compns. for increasing the efficacy
        of biol. -active ingredients such as antitumor agents)
IT
    Bone, neoplasm
     Sarcoma
        (osteosarcoma; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
    Rosin
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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (partially hydrogenated; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
IT
    Citrus limon
        (peel oil; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (pepper, Piper nigrum berry; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (peppermint; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Sulfonic acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (petroleum, sodium salts; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
IT
     Tar
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (pine, oil; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents) .
IT
     Essential oils
     Tar
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (pine; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Rosin
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (polymerized; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Vinyl compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (polymers, synthetic; methods and compns. for increasing the efficacy
        of biol. -active ingredients such as antitumor agents)
     Vinyl compounds, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (polymers; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Malus pumila
        (pomace; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
        (poultry; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Gelatins, biological studies RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (powdered; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Beta vulgaris
        (powder; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
         (product, hydrolyzed; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Carcinoma
        (pulmonary small-cell; methods and compns. for increasing the efficacy
        of biol. -active ingredients such as antitumor agents)
IT
     Citrus sinensis
         (pulp; methods and compns. for increasing the efficacy of biol.-active
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ingredients such as antitumor agents)
     Xanthomonas campestris
         (pv Poannua; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Antitumor agents
         (resistance to; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
         (rhabdomyosarcoma; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Essential oils
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (rosemary; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (rosin; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
    Flours and Meals
        (rye; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Naphthenic acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (salts, compound with dodecyldimethylbenzylammonium; methods and compns.
        for increasing the efficacy of biol. -active ingredients such as
        antitumor agents)
IT
     Sulfonic acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (salts; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (sassafras; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
        (scraps; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Weed
        (seed oil; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Panicum
        (seed; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Bacillus sphaericus
        (serotype H-5A5B, strain 2362; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
     Fats and Glyceridic oils, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (sesame; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Fertilizers
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (sewage sludge; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Egg
        (shell; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Juglans regia
        (shells, ground; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Arachis hypogaea
IT
        (shells; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
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IT
    Lung, neoplasm
        (small-cell carcinoma; methods and compns. for increasing the efficacy
        of biol.-active ingredients such as antitumor agents)
    Caseins, biological studies
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (sodium complexes; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
    Polyphosphoric acids
     Sulfonic acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (sodium salts; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
ΙT
     Soaps
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (sodium tallow; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
ΙT
    Animal tissue, disease
        (soft, neoplasm, sarcoma; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Sarcoma
        (soft-tissue; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Amines, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (soya alkyl, ethoxylated; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)
     Fatty acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (soya, Me esters; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Flours and Meals
        (soybean; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Proteins
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (soybean; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (spearmint; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Fats and Glyceridic oils, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (sperm oil; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Phlebiopsis gigantea
        (spores and mycelium spores; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
     Gliocladium catenulatum
     Nosema locustae
     Paenibacillus popilliae
        (spores; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
    Pseudomonas chlororaphis
         (strain 63-28; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Pseudomonas syringae
        (strain 742 RS; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
ΙT
     Pseudomonas syringae
        (strain AGS31 & strain PS31; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
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(strain BPO; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Pseudomonas syringae
         (strain ESC-10; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Pseudomonas syringae
         (strain ESC-11; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Agrobacterium tumefaciens
         (strain K1026; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Streptomyces griseoviridis
         (strain K61; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Agrobacterium tumefaciens
         (strain K84; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Pseudomonas fluorescens
         (strain NCIB 12089; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Pseudomonas chlororaphis
        (strain Tx-1; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
     Bacillus cereus
         (strain UW85; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
    Hordeum vulgare
        (straw; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (sub Kurstaki strain EG7673 coleopteran active toxin; methods and
        compns. for increasing the efficacy of biol.-active ingredients such as
        antitumor agents)
IT
     Bacillus thuringiensis
        (sub Kurstaki strain EG7673 lepidopteran active toxin; methods and
        compns. for increasing the efficacy of biol.-active ingredients such as
        antitumor agents)
     Bacillus thuringiensis
ΙT
        (subsp Aizawai, GC-91 protein; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (subsp Aizawai, serotype H-7; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
     Bacillus thuringiensis
ΙT
        (subsp Aizawai; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (subsp Israelensis, serotype H-14; methods and compns. for increasing
        the efficacy of biol.-active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (subsp Kurstaki strain SA-12; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (subsp Kurstaki, genetically engineered strain AGRO1 by Agrevo; methods and compns. for increasing the efficacy of biol.-active ingredients
        such as antitumor agents)
1T
     Bacillus thuringiensis
        (subsp Kurstaki, genetically engineered strain AGRO2 by Agrevo; methods and compns. for increasing the efficacy of biol.-active ingredients
        such as antitumor agents)
     Bacillus thuringiensis
IT
        (subsp Kurstaki, serotype; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (subsp Kurstaki, strain EG2348; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (subsp Kurstaki, strain EG2371; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
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IT

Bacillus cereus

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IT
     Bacillus thuringiensis
        (subsp Kurstaki, strain EG2424; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (subsp Kurstaki, strain SA-1 1; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (subsp Morrisoni, serotype 8a8b; methods and compns. for increasing the
        efficacy of biol.-active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
     Bacillus thuringiensis
        (subsp San Diego; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Bacillus thuringiensis
        (subsp Tenebrionis; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
ΙT
     Bacillus thuringiensis
        (subspec Tenebrionis delta endotoxin; methods and compns. for
        increasing the efficacy of biol. -active ingredients such as antitumor
        agents)
     Bacillus thuringiensis
IT
        (subspecies Israelensis strain EG2215; methods and compns. for
        increasing the efficacy of biol.-active ingredients such as antitumor
     Bacillus thuringiensis
IT
         (subspecies Israelensis, strain IPS-78; methods and compns. for
        increasing the efficacy of biol. -active ingredients such as antitumor
IT
     Bacillus thuringiensis
        (subspecies Kurstaki strain HD-1, lepidopteran active toxin; methods
        and compns. for increasing the efficacy of biol.-active ingredients
        such as antitumor agents)
IT
     Bacillus thuringiensis
         (subspecies kurstaki strain BMP 123; methods and compns. for increasing
        the efficacy of biol. -active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (subspecies kurstaki, genetically engineered strain EG7841 lepidopteran active toxin; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Cod liver oil
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (sulfonated; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Petroleum, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (sulfurized; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Helianthus annuus
        (sunflower seed; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
IT
     Seed
        (sunflower; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Fatty acids, biological studies
     Fatty acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (tall-oil, copper salts; methods and compns. for increasing the
        efficacy of biol. -active ingredients such as antitumor agents)
     Fatty acids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (tall-oil; methods and compns. for increasing the efficacy of
        biol. -active ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (thyme, Thymus vulgaris; methods and compns. for increasing the
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efficacy of biol. -active ingredients such as antitumor agents)
     Burkholderia cepacia
IT
         (type Wisconsin; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Petroleum, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (unrefined; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Carcinoma
         (uterine endometrial adenocarcinoma; methods and compns. for increasing
        the efficacy of biol. -active ingredients such as antitumor agents)
IT
     Bacillus thuringiensis
        (var Kurstaki strain M-200 protein toxin; methods and compns. for increasing the efficacy of biol.-active ingredients such as antitumor
        agents)
     Bacillus thuringiensis
IT
         (var Kurstaki, genetically engineered strain ECX; methods and compns.
        for increasing the efficacy of biol. -active ingredients such as
        antitumor agents)
IT
     Bacillus thuringiensis
         (var Kurstaki, genetically engineered strain EG7826 Lepidopteran active
        toxin; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
ΙT
     Bacillus thuringiensis
         (var kurstaki delta endotoxin protein; methods and compns. for
        increasing the efficacy of biol. -active ingredients such as antitumor
        agents)
     Fats and Glyceridic oils, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (vegetable, hydrogenated; methods and compns. for increasing the efficacy of biol.—active ingredients such as antitumor agents)
     Fats and Glyceridic oils, biological studies
     Fats and Glyceridic oils, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (vegetable; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Alkaloids, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (vinca; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
IT
    Dyes
        (water-soluble; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Glycerides, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (wheat germ-oil; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
     Fats and Glyceridic oils, biological studies
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (wheat germ; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
IT
    Pepper (spice)
         (white; methods and compns. for increasing the efficacy of biol.-active
        ingredients such as antitumor agents)
     Essential oils
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (wintergreen; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
    Linseed oil RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (with driers; methods and compns. for increasing the efficacy of
        biol.-active ingredients such as antitumor agents)
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IT
        Creosote
             (wood; methods and compns. for increasing the efficacy of biol.-active
             ingredients such as antitumor agents)
        Naphthenic acids, biological studies
        Naphthenic acids, biological studies
        Resin acids
        Resin acids
        RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
        (Biological study); USES (Uses)
             (zinc salts; methods and compns. for increasing the efficacy of
             biol.-active ingredients such as antitumor agents)
        Interferons
        RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
        (Biological study); USES (Uses)
             (a; methods and compns. for increasing the efficacy of
             biol. -active ingredients such as antitumor agents)
IT
       Lactams
        RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
        (Biological study); USES (Uses)
              (β-; methods and compns. for increasing the efficacy of
             biol.-active ingredients such as antitumor agents)
        74-82-8D, Methane, 11101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 1101,1 110
                                                                      85-86-9, Sudan III
                                                                                                          109-76-2D
                                                                                  115-31-1, Thanite
                                                                                                                     645-92-1
                                                                                       3768-14-7
                                                                                                           4147-57-3
                                                                    8003-19-8D, derivs.
        7206-15-7
                            7206-27-1
                                                8003-06-3
                                                                                                         8064-49-1, Tenox
               8066-01-1
                             8076-84-4, Tenox 4
12770-24-0, Toximul-P
                                                                      9003-01-4
                                                                                          9003-05-8, Polyacrylamide
                                                                                            31895-21-3, Thiocyclam
                                                                      26532-25-2
        11144-43-7
                                                                    37300-16-6, Versalon 1112
        35513-93-0D, N-C6-18alkyl derivs.
                                                                                                                   37350-66-6
        39384-60-6, Tenox S 1 4
51796-19-1, Thixatrol ST
                                                41481-51-0
                                                                      50863-22-4
                                                                                            51068-60-1, Sulglycapin
                                                     51811-79-1, T-Mulz 565
                                                                                               52236-30-3
        52508-35-7
                              58175-59-0
                                                    58175-60-3
                                                                         60864-33-7, Triton CF-10
                                                63100-33-4, Triton X 363
70193-21-4, Trichlamide
        62031-70-3, Wingstay V
                                                                                               66227-09-6
        67053-55-8,
                           Toximul D
                                                                                            72459-58-6, Triazoxide
                                                       76930-44-4, Po-san A
        76608-88-3, Triapenthenol
                                                                                            81412-43-3, Tridemorph
                                          85411-41-2, T-Mulz AO 2 87917-06-4, Tensiofix B
        83869-01-6, TF 310
                  87917-07-5, Tensiofix B 7453 92302-40-4
                                                                                            92529-51-6, Sure-Sol
        7416
                                                            99105-77-8, Sulcotrione
                 94189-31-8, Stepantan A
                                                                                                        103737-35-5,
                          116170-30-0, Thicyofen 118134-30-8, Spiroxamine
        T-Mulz VO
        119515-38-7, Propidine
                                                 123249-43-4, Thidiazimin
                                                                                               130561-48-7, Cintofen
        139963-64-7
                               154201-55-5
                                                       168832-50-6
                                                                              171248-07-0
                                                                                                      291536-79-3
        291536-80-6
                                                       291536-84-0 291536-86-2
                               291536-82-8
        291536-87-3
                               291536-88-4
                                                       291536-89-5
                                                                               291536-90-8
                                                                                                      291536-91-9
                               358622-53-4
        313493-42-4
                                                       403806-37-1
                                                                               845739-24-4
                                                                                                      845739-25-5
        845739-26-6
                               845739-27-7
                                                       845739-28-8
                                                                               845739-29-9
        RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
        (Biological study); USES (Uses)
             (methods and compns. for increasing the efficacy of biol.-active
             ingredients such as antitumor agents)
        9003-18-3
        RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
        (Biological study); USES (Uses)
             (nitrile rubber; methods and compns. for increasing the efficacy of
             biol.-active ingredients such as antitumor agents)
IT
        11121-88-3, Versamid
        RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
             (resin binder; methods and compns. for increasing the efficacy of
             biol.-active ingredients such as antitumor agents)
        291536-86-2
        RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
        (Biological study); USES (Uses)
              (methods and compns. for increasing the efficacy of biol.-active
             ingredients such as antitumor agents)
        291536-86-2 HCAPLUS
        Benzoic acid, 2-[[(4-chlorophenyl)amino]carbonyl]-, 2-propynyl ester (9CI)
CN
           (CA INDEX NAME)
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ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
     2003:23438 HCAPLUS
AN
DN
      138:68713
ED
     Entered STN: 10 Jan 2003
     Modulating resistance of tumor and pathogen cells to foreign compounds by
TI
     manipulation of ATP gradients via regulation of ABC transporters and
      ecto-phosphatases
IN
     Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.
PA
     University of Texas, USA
S<sub>0</sub>
     U.S. Pat. Appl. Publ., 41 pp., Cont.-in-part of U.S. Ser. No. 261,825.
     CODEN: USXXCO
DT
     Patent
LA
     English
      ICM C12N009-12
IC
          C12N009-00
      ICS
INCL 435194000; 435183000
      6-1 (General Biochemistry)
      Section cross-reference (s): 1, 5, 7, 10, 11, 13
FAN. CNT 3
     PATENT NO.
                                                   APPLICATION NO.
                                                                              DATE
                             KIND
                                     DATE
PΙ
     US 2003008369
                              A1
                                      20030109
                                                   US 2002-134019
                                                                               20020425
                                                   US 1999-244792
     US 2002006901
                                      20020117
                                                                               19990205
                              A1
     WO 2003091403
                              A2
                                      20031106
                                                   WO 2003-US12780
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     WO 2003091403
                                     20041104
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PRAI US 1999-244792
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      US 1999-261825
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     US 2002-134019
                              A1
                                     20020425
CLASS
 PATENT NO.
                   CLASS
                            PATENT FAMILY CLASSIFICATION CODES
 US 2003008369
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                            C12N009-12
                            C12N009-00
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                    INCL
                            435194000; 435183000
 US 2003008369
                            435/194.000; 435/183.000
                   NCL
                   ECLA
                            A61K009/00M20B; A61K031/165+A; A61K031/165H;
                            A61K031/165P; A61K031/18; A61K031/215L; A61K031/215L10; A61K031/24; A61K031/35P10; A61K031/38H; A61K031/40T10; A61K031/425F; A61K038/13; A61K038/13+M; C07K014/705;
                            C12N009/14; C12N015/82C8B4
                            514/011.000; 514/009.000; 424/045.000
 US 2002006901
                   NCL
                            A61K009/00M20B; A61K038/13; A61K038/13+M
                   ECLA
     The present invention relates to methods for modulating the growth of
AR
      tumor and pathogen cells and the resistance of cells to foreign compds.,
     i.e. drugs, antibiotics, etc. by altering the ATP gradient across biol. membranes. The altering of the ATP gradient across biol. membranes is achieved through the manipulation of ecto-phosphatase (e.g., human
     apyrase) activity and ABC transporter mol. (e.g., Arabidopsis AtPGP-1)
     activity which may also be useful to confer herbicide resistance to
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plants, confer antibiotic resistance to bacteria, confer drug resistance to yeast cells, or to reduce resistance in cells to facilitate chemotherapeutic treatments, and to reduce resistance in bacteria and yeast. The present invention is also directed to the methods for identifying ecto-phosphatase inhibitors and uses thereof. Nineteen ecto-phosphatase inhibitory mols. are provided which are useful in reversing multi-drug resistance in Arabidopsis and yeast. drug resistance ATP gradient ABC transporter phosphatase; antibiotic

of drug resistance ATP gradient ABC transporter phosphatase; antibiotic resistance ATP gradient ABC transporter phosphatase; herbicide resistance ATP gradient ABC transporter phosphatase; tumor multidrug resistance ATP gradient modulation

IT Transport proteins

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(ABC (ATP-binding cassette) transporters; modulating resistance of
tumor and pathogen cells to foreign compds. by manipulation of ATP
gradients via regulation of ABC transporters and ecto-phosphatases)

IT Neoplasm

(bone marrow; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

IT Intestine, neoplasm

(colon; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

IT Antibiotics

Antitumor agents

Herbicides

(increasing effectiveness of; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

Antibiotic resistance
Bladder, neoplasm
Bone, neoplasm
Brain, neoplasm
Drug resistance
Herbicide resistance

Human

Liver, neoplasm Lung, neoplasm

Lymphoma Mammalia

Mammary gland, neoplasm

Multidrug resistance Ovary, neoplasm

Pancreas, neoplasm Prostate gland, neoplasm

Skin, neoplasm Staphylococcus

Staphylococcus aureus

Stomach, neoplasm

Testis, neoplasm

(modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

IT P-glycoproteins

RL: BSU (Biological study, unclassified); BIOL (Biological study) (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

IT Bone marrow, disease

(neoplasm; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

IT Animal tissue, disease

(soft, neoplasm; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

IT Neoplasm

(soft-tissue; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC

transporters and ecto-phosphatases) 865-21-4. Vinblastine IT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (increasing effectiveness of; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

61-32-5, Methicillin RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (inhibiting growth of cells resistant to; modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

171248-07-0 168832-50-6 IT 41481-51-0 139963-64-7 154201-55-5 291536-80-6 291536-81-7 291536-79-3 291536-82-8 291536-84-0 291536-85-1 **291536-86-2** 291536-87-3 291536-88-4 291536-89-5 · 291536-90-8 291536-91-9 **291536-92-0** 313493-42-4

RL: AGR (Agricultural use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

56-65-5, 5'-ATP, biological studies 9000-95-7, Apyrase Phosphatase

RL: BSU (Biological study, unclassified); BIOL (Biological study) (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

291536-86-2 IT

RL: AGR (Agricultural use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (modulating resistance of tumor and pathogen cells to foreign compds. by manipulation of ATP gradients via regulation of ABC transporters and ecto-phosphatases)

RN

291536-86-2 HCAPLUS
Benzoic acid, 2-[[(4-chlorophenyl)amino]carbonyl]-, 2-propynyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \text{C1} \\ \hline & \text{C-NH} & & & \text{C1} \\ \hline & \text{C-O-CH}_2\text{-C} & & \text{CH} \\ \end{array}$$

ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN L50

2002:833490 HCAPLUS AN

DN 137:306061

Entered STN: 01 Nov 2002 ED

Pesticidal and herbicidal activity through modulation of animal and plant ΤI cell membrane transport

IN Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M. Board of Regents, The University of Texas System, USA

S₀ U.S. Pat. Appl. Publ., 41 pp., Cont.-in-part of U.S. Ser. No. 244,791.

CODEN: USXXCO

DT Patent

LA English

ICM A01N025-00 IC

INCL 504116100

5-4 (Agrochemical Bioregulators)

FAN.	CNT 3 PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	US 2002160915	A1	20021031	US 2001-793336	20010226
	US 6448472	B1	20020910	US 1999-244791	19990205
PRAI	US 1999-244791	A2	19990205		•

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US 2000-185299P
                                   20000228
CLASS
PATENT NO.
                          PATENT FAMILY CLASSIFICATION CODES
                   CLASS
US 2002160915
                           A01N025-00
                   ICM
                   INCL
                           504116100
US 2002160915
                          504/116.100
                   NCL
                   ECLA
                          A01N037/28; A01N037/30; A01N061/00; C07K014/415;
                          C12N009/14; C12N015/82C4B; C12N015/82C8B4;
                           C12N015/82C8B; C12Q001/42
                           800/278.000; 435/320.100; 435/418.000; 435/419.000;
US 6448472
                   NCL
                           435/468.000; 800/298.000; 800/300.000
                   ECLA
                          C07K014/415; C12N009/14; C12N015/82C8B4
AB
     The present invention relates to the modulation of pesticidal and
     herbicidal activity by treatment of a membrane transport system in a cell.
     This entails modifying the extra-cellular phosphatases found in the
     membranes of these cells. By modifying the ATP gradient across the biol.
     membrane of a target plant, bacteria, insect or mammalian cell via
     inhibiting one or more extra-cellular phosphatases, it is possible to
     alter the sensitivity to a pesticide or herbicide. The method also comprises inhibiting an ABC transporter in the target cell. The method can also be used for identifying chems. with pesticidal activity.
     pesticidal herbicidal activity modulation animal plant plasma membrane
     transport; pesticide herbicide ectophosphatase ABC transporter inhibition
     Transport proteins
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (ABC (ATP-binding cassette) transporters; enhancement of pesticidal and
         herbicidal activity by altering the ATP gradient across biol. membranes
         and inhibiting an ABC transporter)
     Herbicides
TI
     Pesticides
         (ectophosphatase inhibitors which enhance pesticidal and herbicidal
         activity by altering the ATP gradient across biol. membranes)
IT
     Pesticides
         (toxicity; ectophosphatase inhibitors which enhance pesticidal and
         herbicidal activity by altering the ATP gradient across biol.
         membranes)
     41481-51-0
                   139963-64-7
                                   154201-55-5
                                                   168832-50-6
                                                                   171248-07-0
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     291536-79-3
                     291536-80-6
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                                                                    291536-83-9
     291536-84-0 291536-86-2
                                   291536-87-3
                                                   291536-88-4
     291536-89-5
                                    291536-91-9 291536-92-0
                     291536-90-8
     358622-53-4
     RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL
     (Biological study); USES (Uses)
         (ectophosphatase inhibitor which enhances pesticidal and herbicidal
         activity by altering the ATP gradient across biol. membranes)
     56-65-5, ATP, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
IT
         (ectophosphatase inhibitors which enhance pesticidal and herbicidal
         activity by altering the ATP gradient across biol. membranes)
     9032-64-8, Nucleotide pyrophosphatase 37289-25-1, ATP pyrophosphatase RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (extracellular; ectophosphatase inhibitors which enhance pesticidal and
         herbicidal activity by altering the ATP gradient across biol.
         membranes)
IT
     291536-86-2
     RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL
     (Biological study); USES (Uses)
        (ectophosphatase inhibitor which enhances pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes)
     291536-86-2 HCAPLUS
RN
     Benzoic acid, 2-[[(4-chlorophenyl)amino]carbonyl]-, 2-propynyl ester (9CI)
CN
        (CA INDEX NAME)
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L50 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
      2002:185280 HCAPLUS
AN
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      136:244034
ED
      Entered STN: 15 Mar 2002
ΤI
      Method for increasing the effectiveness of antiinfective agents by
      inhibiting ecto-phosphatase and/or ABC transporter activities Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M. Board of Regents, the University of Texas System, USA
IN
PA
      PCT Int. Appl., 65 pp.
S0
      CODEN: PIXXD2
DT
      Patent
      English
LA
      ICM C12N
9-12 (Biochemical Methods)
IC
      Section cross-reference(s): 1, 5, 7, 10, 11
FAN. CNT 1
      PATENT NO.
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                                                     APPLICATION NO.
                                                                                 DATE
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PRAI US 2000-231088P
WO 2001-US28242
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                                       20010907
CLASS
                             PATENT FAMILY CLASSIFICATION CODES
 PATENT NO.
                     CLASS
 WO 2002020726
                     ICM
 US 2002077365
                     NCL
                             514/621.000; 504/329.000; 514/553.000; 504/149.000
                             A01N037/10; A01N037/22; A01N037/28; A01N037/28+M; A01N037/30; A01N037/38; A01N037/46; A01N041/06; A01N043/12; A01N043/16; A01N043/38; A01N043/78;
                     ECLA
                             A01N047/06; A01N047/30; A01N047/44; A61K031/185;
                             C12N009/14; C12N015/82C8; C12N015/82C8B4
GI
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AB The present invention relates to methods for decreasing the resistance of microbial strains to antiinfectives such an antibiotics and antifungals by altering the ATP gradient across biol. membranes. The altering of the ATP gradient across biol. membranes is achieved through the inhibition of ecto-phosphatase activity and/or ABC transporter mol. activity which may be useful to reduce resistance in bacteria and yeast to aid in the treatment of certain infections and disease and to lower the concentration of antiinfectives necessary to inhibit the growth of microbial strains. Apyrase inhibitor I increased the growth inhibitory effect of the fungicide chlorothalonil by over 50%. Surflan was an equally effective weed killer against Arabidopsis thaliana at a five-fold less concentration in the presence of II.

ST antiinfective enhancement inhibition ectophosphatase ABC transporter; ATP gradient biol membrane antibiotic antifungal effectiveness; yeast bacteria resistance ectophosphatase ABC transporter; chlorothalonil fungicide enhancement apyrase inhibitor; surflan herbicide adjuvant apyrase inhibitor

IT Transport proteins

RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); BIOL (Biological study)

(ABC (ATP-binding cassette) transporters; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities)

Gene, plant

RL: BPN (Biological study): PREP (Preparation);

BIOL (Biological study); PREP (Preparation)

(AtPGP-1; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities) Combinatorial library

(DIVERSet format F, high throughput screening for apyrase inhibitors; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities)

T P-glycoproteins

RL: ADV (Adverse effect, including toxicity); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation)

(MDR1; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities)

IT Agrochemical formulations

(adjuvants; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities)

IT Fungicides

(agrochem.; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities)

IT Membrane, biological

(altering ATP gradient across; method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities)

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ΙT
    Plant cell
        (as target cell; method for increasing effectiveness of antiinfective
        agents by inhibiting ecto-phosphatase and/or ABC transporter
        activities)
IT
     Infection
        (bacterial; method for increasing effectiveness of antiinfective agents
        by inhibiting ecto-phosphatase and/or ABC transporter activities)
IT
    High throughput screening
        (drug, for apyrase inhibitors; method for increasing effectiveness of
        antiinfective agents by inhibiting ecto-phosphatase and/or ABC
        transporter activities)
     Biological transport
        (efflux; method for increasing effectiveness of antiinfective agents by
        inhibiting ecto-phosphatase and/or ABC transporter activities)
IT
     Gene, plant
     RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified);
     BIOL (Biological study); PREP (Preparation)
        (for apyrase; method for increasing effectiveness of antiinfective
        agents by inhibiting ecto-phosphatase and/or ABC transporter
        activities)
IT
     Drug screening
        (high throughput, for apyrase inhibitors; method for increasing
        effectiveness of antiinfective agents by inhibiting ecto-phosphatase
        and/or ABC transporter activities)
     Anti-infective agents
        (medical; method for increasing effectiveness of antiinfective agents
        by inhibiting ecto-phosphatase and/or ABC transporter activities)
IT
     Acaricides
     Algicides
     Animal
     Anti-infective agents
     Antibacterial agents
     Antibiotic resistance
     Antibiotics
     Antimicrobial agents
     Arabidopsis thaliana
     Bactericide resistance
     Drug delivery systems
     Drug resistance
     Embryophyta
     Eubacteria
     Fungicide resistance
     Fungicides
     Herbicide resistance
     Herbicides
     Human
     Insecticides
     Mammalia
     Multidrug resistance
     Nematocides
     Pesticides
     Pisum sativum
     Saccharomyces cerevisiae
     Yeast
        (method for increasing effectiveness of antiinfective agents by
        inhibiting ecto-phosphatase and/or ABC transporter activities)
    Multidrug resistance proteins
     RL: ADV (Adverse effect, including toxicity); BPN (Biosynthetic
     preparation); BSU (Biological study, unclassified); BIOL (Biological
     study); PREP (Preparation)
        (method for increasing effectiveness of antiinfective agents by
        inhibiting ecto-phosphatase and/or ABC transporter activities)
IT
    Pesticides
        (toxicity; method for increasing effectiveness of antiinfective agents
        by inhibiting ecto-phosphatase and/or ABC transporter activities)
IT
     Infection
        (yeast; method for increasing effectiveness of antiinfective agents by
        inhibiting ecto-phosphatase and/or ABC transporter activities)
     56-65-5, 5'-ATP, biological studies RL: BSU (Biological study, unclassified); CUS (Combinatorial use); BIOL
IT
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(Biological study); CMBI (Combinatorial study); USES (Uses)
         (altering gradient of, across biol. membrane; method for increasing
         effectiveness of antiinfective agents by inhibiting ecto-phosphatase
         and/or ABC transporter activities)
IT
     41481-51-0
                  139963-64-7
                                   154201-55-5
                                                    168832-50-6
                                                                    171248-07-0
                     291536-81-7
     291536-79-3
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                                     291536-89-5
                                                     291536-90-8
                     291536-88-4
     313493-42-4
                     403806-37-1
     RL: BSU (Biological study, unclassified); CST (Combinatorial study,
     unclassified); BIOL (Biological study); CMBI (Combinatorial study)
         (as apyrase inhibitor; method for increasing effectiveness of
         antiinfective agents by inhibiting ecto-phosphatase and/or ABC
         transporter activities)
     9000-95-7, Apyrase
IT
     RL: ADV (Adverse effect, including toxicity); BSU (Biological study,
     unclassified); CUS (Combinatorial use); BIOL (Biological study); CMBI
      (Combinatorial study); USES (Uses)
         (ecto-; method for increasing effectiveness of antiinfective agents by
         inhibiting ecto-phosphatase and/or ABC transporter activities)
     9000-83-3, ATPase
IT
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (inhibition of, of ectophosphatase; method for increasing effectiveness
         of antiinfective agents by inhibiting ecto-phosphatase and/or ABC
         transporter activities)
     19044-88-3, Surflan 40487-42-1, Pendimethalin RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL.
      (Biological study); USES (Uses)
         (method for increasing effectiveness of antiinfective agents by
         inhibiting ecto-phosphatase and/or ABC transporter activities)
     291536-80-6 291536-85-1
IT
     RL: AGR (Agricultural use); DMA (Drug mechanism of action); BIOL
      (Biological study); USES (Uses)
         (method for increasing effectiveness of antiinfective agents by
         inhibiting ecto-phosphatase and/or ABC transporter activities)
IT
     145-63-1, Suramin
     RL: AGR (Agricultural use); DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological
     study); USES (Uses)
         (method for increasing effectiveness of antiinfective agents by
     inhibiting ecto-phosphatase and/or ABC transporter activities) 66-81-9, Cycloheximide 2365-40-4, N6-(2-Isopentenyl)adenine 3 α, β-Methyleneadenosine 5'-diphosphate 28380-24-7, Nigericin
                                                                              3768-14-7,
IT
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (method for increasing effectiveness of antiinfective agents by inhibiting ecto-phosphatase and/or ABC transporter activities)
     1897-45-6, Chlorothalonil
     RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (method for increasing effectiveness of antiinfective agents by
         inhibiting ecto-phosphatase and/or ABC transporter activities)
     291536-86-2
IT
     RL: BSU (Biological study, unclassified); CST (Combinatorial study,
     unclassified); BIOL (Biological study); CMBI (Combinatorial study)
         (as apyrase inhibitor; method for increasing effectiveness of
         antiinfective agents by inhibiting ecto-phosphatase and/or ABC
         transporter activities)
     291536-86-2 HCAPLUS
RN
CN
     Benzoic acid, 2-[[(4-chlorophenyl)amino]carbonyl]-, 2-propynyl ester (9CI)
        (CA INDEX NAME)
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ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
L50
     2001:676991 HCAPLUS
     135:222868
     Entered STN: 14 Sep 2001
ED
ΤI
     Pesticide adjuvant activity through modulation of animal and plant cell
     membrane transport
     Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.
     Board of Regents of the University of Texas System, USA
PA
SO
     PCT Int. Appl., 76 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LA
IC
     ICM C12Q001-42
          C12Q001-34; C12Q001-00
     ICS
     5-4 (Agrochemical Bioregulators)
FAN. CNT 1
     PATENT NO.
                          KIND
                                  DATE
                                              APPLICATION NO.
                                                                       DATE
                                                                       20010307
PΙ
     WO 2001066792
                           A1
                                  20010913
                                              WO 2001-US7423
         W: AE, AG,
                          AM, AT, AU,
                                      AZ, BA,
                                               BB, BG, BR, BY, BZ,
                                                                    CA,
                                                                        CH, CN,
                     AL.
                                                                GE,
             CR, CU,
                      CZ,
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             HU. ID.
                     IL,
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                                       KE,
                                               KP, KR,
                                                            LC,
                                                                    LR, LS, LT,
                                           KG,
                                           MW, MX, MZ,
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             LU, LV,
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                                  MK,
                                       MN,
                                                                    PT,
                                                                        RO, RU,
                              SK,
                                               TR,
             SD,
                                  SL,
                                      TJ,
KZ,
                 SE,
                      SG,
                          SI,
                                           TM,
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                                                        TZ.
                                                            UA, UG,
                                                                    UZ,
                                                                        VN, YU,
                 ZW,
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                              BY,
              ZA,
                          AZ,
                                  KG,
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                                               RU,
                                                   TJ,
                                                        TM
                                               SZ,
         RW: GH, GM, KE, LS,
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                                                   TZ,
                                                       UG, ZW, AT,
                                  MZ,
                                      SD,
                                           SL,
                                                                    BE, CH, CY,
                                                       MC, NL, PT,
                      ES, FI, FR,
                                  GB, GR,
             DE, DK,
                                           IE, IT, LU,
                                                                    SE,
                                                                        TR, BF,
                                           GW,
                                              ML, MR, NE, SI
US 2001-800327
                 CF,
                     CG,
                              CM,
                                  GA,
                                      GN,
                                                            SN,
                                                               TD,
                                                                    TG
             BJ,
                          CI,
     US 2002103082
                                  20020801
                                                                       20010306
                           A1
     CA 2373424
                                  20010913
                                              CA 2001-2373424
                                                                       20010307
                           AA
PRAI US 2000-187819P
US 2001-800327
                           P
                                  20000308
                                  20010306
                           A
     WO 2001-US7423
                                  20010307
CLASS
 PATENT NO.
                  CLASS
                         PATENT FAMILY CLASSIFICATION CODES
 WO 2001066792
                  ICM
                         C12Q001-42
                         C12Q001-34; C12Q001-00
                  ICS
 US 2002103082
                 NCL
                         504/116.100; 504/117.000
                         C12Q001/42
                  ECLA
     The invention relates to the modulation of pesticidal and herbicidal
     activity by treatment of a membrane transport system in a cell. This
     entails modifying the extracellular phosphatases found in the membranes of
     these cells. By modifying the ATP gradient across the biol. membrane of a
     target plant, bacteria, insect or mammalian cell via inhibiting one or
     more extracellular phosphatases, it is possible to alter the sensitivity
     to a pesticide or herbicide. In preferred embodiments, the chemical moieties
     of the invention act as adjuvants to enhance pesticidal activity.
     pesticide adjuvant membrane extracellular phosphatase inhibition
     Transport proteins
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
         (ABC (ATP-binding cassette-containing); pesticide adjuvants acting by
        inhibition of extracellular phosphatases and ABC transporters)
IT
     Fungicides
         (fungicide adjuvants acting by inhibition of extracellular phosphatases
        in membranes)
ΙT
     Herbicides
        (herbicide adjuvants acting by inhibition of extracellular phosphatases
        in membranes)
IT
     Pesticides
         (pesticide adjuvants acting by inhibition of extracellular phosphatases
        in membranes)
IT
     9013-05-2, Phosphatase
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
         (ecto-; pesticide adjuvants acting by inhibition of extracellular
        phosphatases in membranes)
IT
     1897-45-6, Chlorothalonil
```

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RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
   (fungicide adjuvants acting by inhibition of extracellular phosphatases
   in membranes)
19044-88-3, Surflan 40487-42-1, Pendimethalin
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
   (herbicide adjuvants acting by inhibition of extracellular phosphatases
```

in membranes) 139963-64-7 171248-07-0 41481-51-0 154201-55-5 168832-50-6 291536-80-6 291536-82-8 291536-84-0 291536-79-3 291536-81-7 291536-88-4 291536-85-1 **291536-86-2** 291536-87-3 291536-89-5 291536-90-8 291536-91-9 291536-92-0 313493-42-4

RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses) (pesticide adjuvant acting by inhibition of extracellular phosphatases in membranes)

56-65-5, ATP, biological studies RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(pesticide adjuvants acting by modification of ATP gradients across membranes)

RE. CNT THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD RE

Boyum; Biochem Biophys Res Commun 1997, V230, P22 HCAPLUS (1)

Decottignies; J Biol Chem 1998, V273 (20), P12612 HCAPLUS Grant; Cancer Research 1994, V54, P357 HCAPLUS Thomas; The Plant Cell 2000, V12, P519 HCAPLUS (4)

(5) University Of Texas; WO 0052144 A1 2000 HCAPLUS 291536-86-2 IΤ

RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses) (pesticide adjuvant acting by inhibition of extracellular phosphatases in membranes)

RN 291536-86-2 HCAPLUS

ΙT

CN Benzoic acid, 2-[[(4-chlorophenyl)amino]carbonyl]-, 2-propynyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \text{C1} \\ \hline & & & \\ \text{C-O-CH}_2\text{-C} & \text{CH} \\ \end{array}$$

L50 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

2001:661570 HCAPLUS AN

DN 135:206922

Entered STN: 10 Sep 2001 ED

ΤI Pesticidal and herbicidal activity through modulation of animal and plant cell membrane transport

IN Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M. Board of Regents, the University of Texas System, USA PA

S0 PCT Int. Appl., 74 pp. CODEN: PIXXD2

DT Patent

LA English

IC C12N009-99; C12N015-01; A01H001-06

5-4 (Agrochemical Bioregulators)

FAN. CNT 3

	PATENT NO. WO 2001064859				KIND DATE			APPLICATION NO.						DATE				
ΡI				A1 20010907		WO 2001-US6503						20010227						
		₩:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
			CR.	CU,	CZ.	DE.	DK.	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,
								JP,										
								MK,										
			SD,	SE.	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	UZ,	VN,	YU,
								KĠ,							,			

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI US 2000-185299P
                                  20000228
CLASS
PATENT NO.
                  CLASS PATENT FAMILY CLASSIFICATION CODES
WO 2001064859
                  IC
                         C12N009-99IC
                                            C12N015-01IC
                                                              A01H001-06
    The invention relates to the modulation of pesticidal and herbicidal
    activity by treatment of a membrane transport system in a cell. This
     entails modifying the extra-cellular phosphatases found in the membranes
     of these cells. By modifying the ATP gradient across the biol. membrane
     of a target plant, bacteria, insect or mammalian cell via inhibiting one
     or more extracellular phosphatases, it is possible to alter the
     sensitivity to a pesticide or herbicide. The method also comprises
     inhibiting an ABC transporter in the target cell. The method can also be
     used for identifying chems. with pesticidal activity.
     pesticide herbicide ectophosphatase ABC transporter inhibition
     Transport proteins
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (ABC (ATP-binding cassette-containing); enhancement of pesticidal and
        herbicidal activity by altering the ATP gradient across biol. membranes
        and inhibiting an ABC transporter)
IT
     Herbicides
     Pesticides
         (ectophosphatase inhibitors which enhance pesticidal and herbicidal
        activity by altering the ATP gradient across biol. membranes)
                                 154201-55-5
                                                                171248-07-0
     41481-51-0
                   139963-64-7
                                                 168832-50-6
                    291536-80-6
     291536-79-3
                                  291536-81-7
                                                  291536-82-8
                                                                 291536-83-9
                                                 291536-88-4
     291536-84-0 291536-86-2
                                 291536-87-3
                    291536-90-8
                                   291536-91-9 291536-92-0
     291536-89-5
     358622-53-4
     RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL
     (Biological study); USES (Uses)
        (ectophosphatase inhibitor which enhances pesticidal and herbicidal activity by altering the ATP gradient across biol. membranes)
     56-65-5, ATP, biological studies
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
        (ectophosphatase inhibitors which enhance pesticidal and herbicidal
        activity by altering the ATP gradient across biol. membranes)
     9032-64-8, Nucleotide pyrophosphatase 37289-25-1, ATP pyrophosphatase
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
         (extracellular; ectophosphatase inhibitors which enhance pesticidal and
        herbicidal activity by altering the ATP gradient across biol.
        membranes)
RE. CNT 2
               THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Lu, Y; The Plant Cell 1998, V10, P267 HCAPLUS
(2) Thomas, C; The Plant Cell 2000, V12, P519 HCAPLUS
     291536-86-2
     RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL
     (Biological study); USES (Uses)
        (ectophosphatase inhibitor which enhances pesticidal and herbicidal
        activity by altering the ATP gradient across biol. membranes)
     291536-86-2 HCAPLUS
RN
CN
     Benzoic acid, 2-[[(4-chlorophenyl)amino]carbonyl]-, 2-propynyl ester (9CI)
       (CA INDEX NAME)
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L50 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
     2000:628251 HCAPLUS
AN
DN
     133:219782
ED
     Entered STN: 10 Sep 2000
     Genetic and epigenetic manipulation of ABC transporters and
     ecto-phosphatases for modulating drug resistance and methods for detection
     of ecto-phosphatase inhibitors
     Thomas, Collin E.; Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.; Hurley, Laurence
IN
     University of Texas, USA
PA
S0
     PCT Int. Appl., 85 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LA
IC
     ICM C12N005-04
          C12N005-06; C12N001-16; C12N001-20; C12N015-67; C12N015-81; C12N015-82; C12N015-90; A01H001-00; A01H005-00
     9-2 (Biochemical Methods)
     Section cross-reference(s): 1, 3, 10, 11
FAN. CNT 3
     PATENT NO.
                           KIND
                                   DATE
                                                APPLICATION NO.
                                                                          DATE
PΙ
     WO 2000052144
                                   20000908
                                                                          20000228
                            A1
                                                 WO 2000-US5315
         W:
             AE, AL,
                      AM,
                           AT, AU, AZ,
                                        BA, BB,
                                                 BG, BR, BY, CA,
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                           DM, EE,
              CZ, DE, DK,
                                    ES,
                                        FI, GB,
                                                 GD, GE, GH, GM, HR, HU, ID, IL,
              IN, IS,
                           KE, KG,
                                    KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
                                                 PL,
                                                      PT,
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              MD, MG,
                      MK,
                           MN,
                               MW,
                                    MX,
                                        NO, NZ,
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                                                                   SD,
                                                                        SE,
                                                                                SI.
                               TR,
              SK,
                  SL,
                       TJ,
                           TM,
                                    TT,
                                        TZ, UA,
                                                 UG,
                                                      UZ,
                                                          VN,
                                                               YU,
                                                                   Z₩,
                                                                       AM,
                                                                                BY,
                      MD,
              KG, KZ,
                           RU, TJ,
                                    TM
                               MW, SD, SL, SZ, TZ, UG, ZW, AT, GB, GR, IE, IT, LU, MC, NL, PT, GN, GW, ML, MR, NE, SN, TD, TG
         RW: GH, GM,
                      KE,
                           LS, MW,
                                                                   BE,
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              DK, ES,
                      FI,
                                                                   SE, BF, BJ, CF,
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              CG,
                           GA,
     EP 1185623
                                   20020313
                                                EP 2000-913685
                            A1
                           DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             AT, BE, CH,
                          LV,
A1
              IE.
                 SI, LT,
                               FI,
                                   RO
     US 2002173031
                                   20021121
                                                US 2002-47251
                                                                          20020114
PRAI US 1999-261825
                            A
                                   19990303
     WO 2000-US5315
                                   20000228
CLASS
PATENT NO.
                  CLASS
                          PATENT FAMILY CLASSIFICATION CODES
WO 2000052144
                  ICM
                          C12N005-04
                          C12N005-06; C12N001-16; C12N001-20; C12N015-67;
                  ICS
                          C12N015-81; C12N015-82; C12N015-90; A01H001-00;
                          A01H005-00
US 2002173031
                  NCL
                          435/245.000; 435/195.000
                  ECLA
                          A61K031/165+A; A61K031/166; A61K031/167; A61K031/18;
                          A61K031/215L10; A61K031/216; A61K031/24; A61K031/352;
                          A61K031/381; A61K031/404; A61K031/425F; C07K014/705; C12N009/14; C12N015/82C8B4
AB
     The present invention relates to methods for modulating the resistance of
     cells to foreign compds., i.e. drugs, antibiotics, etc. by altering the ATP gradient across biol. membranes. Altering the ATP gradient across
     biol. membranes is achieved through the manipulation of ecto-phosphatase
     activity and ABC transporter mol. activity. The above method may be
     useful to confer herbicide resistance to plants, antibiotic resistance to
     bacteria, and drug resistance to yeast cells, or to reduce resistance in
     cells, bacteria, and yeast in order to facilitate chemotherapeutic
     treatments. The present invention is also directed to the methods for
     identifying ecto-phosphatase inhibitors and uses thereof. Thus,
     Arabidopsis thaliana has been shown to possess an ecto-apyrase and this
     ecto-apyrase and PGP-1 (an MDR-like protein) to have a role in MDR.
     Addnl., the extracellular ATP pool was shown to be critical for MDR in yeast.
     Screening of a combinatorial library of small mols. has resulted in
     identification of apyrase inhibitors.
     drug resistance ectophosphatase ABC transporter ATP gradient
ΙT
     Transport proteins
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
```

```
study, unclassified); BIOL (Biological study)
           (ABC; genetic and epigenetic manipulation of ABC transporters and
          ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
  IT
       Membrane, biological
           (ATP gradient across; genetic and epigenetic manipulation of ABC
          transporters and ecto-phosphatases for modulating drug resistance and
          methods for detection of ecto-phosphatase inhibitors)
. IT
       Chemotherapy
       Herbicide resistance
           (augmentation of; genetic and epigenetic manipulation of ABC
          transporters and ecto-phosphatases for modulating drug resistance and
          methods for detection of ecto-phosphatase inhibitors)
  IT
       Neoplasm
           (decreasing drug resistance in; genetic and epigenetic manipulation of
          ABC transporters and ecto-phosphatases for modulating drug resistance
          and methods for detection of ecto-phosphatase inhibitors)
  IT
       Arabidopsis thaliana
       Aspergillus fumigatus
       Bacteria (Eubacteria)
       Drug resistance
       Lactococcus lactis
       Pea
       Plant cell
       Saccharomyces cerevisiae
       Yeast
           (genetic and epigenetic manipulation of ABC transporters and
          ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
  IT
       Animal cell
           (mammalian; genetic and epigenetic manipulation of ABC transporters and
          ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
       50-81-7, Ascorbic acid, uses 11098-84-3, Ammonium molybdate
  IT
       RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
           (genetic and epigenetic manipulation of ABC transporters and
          ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
                                                                154201-55-5
       9013-05-2, Phosphatase 41481-51-0 139963-64-7
  IT
       168832-50-6
                      171248-07-0
                                     291536-79-3
                                                     291536-80-6
                                                                    291536-81-7
       291536-82-8
                                                     291536-85-1 291536-86-2
                      291536-83-9
                                      291536-84-0
       291536-87-3
                      291536-88-4
                                     291536-89-5
                                                     291536-90-8
                                                                   291536-91-9
       291536-92-0
       RL: BAC (Biological activity or effector, except adverse); BSU (Biological
       study, unclassified); BIOL (Biological study)
           (genetic and epigenetic manipulation of ABC transporters and
          ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
  IT
       56-65-5, ATP, biological studies
       RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
       BIOL (Biological study); OCCU (Occurrence)
           (gradient of; genetic and epigenetic manipulation of ABC transporters
          and ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
  RE. CNT 8
                 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
  RE
  (1) Decottignies; J Biol Chem 1998, V273(20), P12612 HCAPLUS
(2) Dudler; J Biol Chem 1992, V267(9), P5882 HCAPLUS
(3) Grant; Cancer Research 1994, V54, P357 HCAPLUS
  (4) Kiba; Plant Cell Physiol 1995, V36(5), P809 HCAPLUS
(5) Lu; The Plant Cell 1998, V10, P267 HCAPLUS
      Sidler; The Plant Cell 1998, V10(10), P1632
Thomas; Plant Physiol 1999, V119, P543 HCAPLUS
      Wang; J Biol Chem 1996, V271(17), P9898 HCAPLUS
       291536-86-2
       RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
           (genetic and epigenetic manipulation of ABC transporters and
          ecto-phosphatases for modulating drug resistance and methods for
          detection of ecto-phosphatase inhibitors)
```

RN 291536-86-2 HCAPLUS CN Benzoic acid, 2-[(4-chlorophenyl)amino]carbonyl]-, 2-propynyl ester (9CI) (CA INDEX NAME)

=> d all hitstr 151 tot L51 ANSWER 1 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN 1999:98011 HCAPLUS AN DN 130:237254 ED Entered STN: 15 Feb 1999 Self-Assembly of Hydrogen-Bonded Polymeric Rods Based on the Cyanuric Acid Melamine Lattice Choi, Insung S.; Li, Xinhua; Simanek, Eric E.; Akaba, Ryoichi; Whitesides, George M. CS Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA Chemistry of Materials (1999), 11(3), 684-690 S₀ CODEN: CMATEX; ISSN: 0897-4756 PR American Chemical Society DT Journal English CC 22-13 (Physical Organic Chemistry) Section cross-reference(s): 35 This paper describes the self-assembly of hydrogen-bonded polymeric rods based on the lattice of cyanuric acid and melamine (CA·M). Data from 1H NMR spectroscopy, IR spectroscopy, gel permeation chromatog. (GPC), and transmission electron microscopy (TEM) are interpreted as indicating that the self-assembly of a bisisocyanuric acid (bisCA) and a

bismelamine (bisM) formed polymeric nanorods [(bisCA)n(bisM)n] composed of parallel CA·M rosettes. The TEM results suggest that these rods aggregate as bundles. The length of the bundles ranged from 100 to 1500 nm, and their diameter was in the range from 15 to 500 nm.

cyanuric acid melamine hydrogen bonded polymeric nanorod self assembly

IR spectroscopy

(Fourier-transform, for aggregate characterization; self-assembly of hydrogen-bonded polymeric rods based on the cyanuric acid melamine lattice)

IT Gel permeation chromatography

Proton NMR spectroscopy

Transmission electron microscopy

(for aggregate characterization; self-assembly of hydrogen-bonded polymeric rods based on the cyanuric acid melamine lattice)

Solvent effect IT

(on aggregate size and morphol.; self-assembly of hydrogen-bonded polymeric rods based on the cyanuric acid melamine lattice)

TT Van der Waals potential

(rod bundles formed by van der Waals interaction between lauryloxypropyl chains; self-assembly of hydrogen-bonded polymeric rods based on the cyanuric acid melamine lattice)

IT Aggregation

Gels

Hydrogen bond

Nanoparticles Self-assembly

(self-assembly of hydrogen-bonded polymeric rods based on the cyanuric acid melamine lattice)

129001-73-6 IT 146651-79-8

RL: PEP (Physical, engineering or chemical process); PRP (Properties);

```
PROC (Process)
               (polymer component; self-assembly of hydrogen-bonded polymeric rods
              based on the cyanuric acid melamine lattice)
         221246-86-2P 221246-89-5P 221246-91-9P
         RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN
         (Synthetic preparation); PREP (Preparation); PROC (Process)
               (preparation as polymer component; self-assembly of hydrogen-bonded
              polymeric rods based on the cyanuric acid melamine lattice)
         108-77-0, Cyanuric chloride 582-16-1, 2,7-Dimethylnaphthalene
IT
         1889-05-0 7617-74-5 16326-62-8, Nitrobiuret RL: RCT (Reactant); RACT (Reactant or reagent)
               (self-assembly of hydrogen-bonded polymeric rods based on the cyanuric
              acid melamine lattice)
         38309-89-6P, 2,7-Bis (bromomethyl) naphthalene 221246-93-1P.
         2, 7-Bis (azidomethyl) naphthalene 221246-95-3P, 2, 7-
         Bis (aminomethyl) naphthalene 221246-96-4P
         RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
         (Reactant or reagent)
               (self-assembly of hydrogen-bonded polymeric rods based on the cyanuric
              acid melamine lattice)
RE. CNT
                        THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Billmeyer, F; Textbook of Polymer Science 1984
(2) Branda, N; Science 1994, V263, P1267 HCAPLUS
(3) Chin, N; J Org Chem 1997, V62, P1891
(4) Clark, T; J Am Chem Soc 1998, V120, P651 HCAPLUS
(5) Ghadiri, M; Adv Mater 1995, V7, P675
(6) Ghadiri, M; Nature 1993, V366, P324 HCAPLUS
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129001-73-6

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(polymer component; self-assembly of hydrogen-bonded polymeric rods based on the cyanuric acid melamine lattice)
129001-73-6 HCAPLUS

1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \text{NH-CH}_2\text{-CH}_2\text{-CMe}_3 \\ \text{NH-CH}_2\text{-CM}_2\text{-CMe}_3 \\ \text{NH-CH}_2\text{-CM}_2\text{-CMe}_3 \\ \text{NH-CH}_2\text{-CM}_2\text{-CMe}_3 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2 \\ \text{NH-CH}_2\text{-CM}_2 \\ \text{NH-CH}_2$$

PAGE 2-A

PAGE 3-A

$$\begin{array}{c} & & & \\ & &$$

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ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     1998:16466 HCAPLUS
DN
     128:29651
     Entered STN: 13 Jan 1998
ED
ΤI
     Self-Assembly of Zinc Porphyrins around the Periphery of Hydrogen-Bonded
     Aggregates That Bear Imidazole Groups
     Simanek, Eric E.; Isaacs, Lyle; Li, Xinhua; Wang, Clay C. C.; Whitesides,
     George M.
     Department of Chemistry and Chemical Biology, Harvard University,
     Cambridge, MA, 02138, USA
     Journal of Organic Chemistry (1997), 62(26), 8994-9000
S<sub>0</sub>
     CODEN: JOCEAH; ISSN: 0022-3263
PB
     American Chemical Society
DT
     Journal
     English
LA
     78-7 (Inorganic Chemicals and Reactions)
     Section cross-reference(s): 28
     This paper describes the preparation and characterization of four aggregates
     that are based on the rosette of derivs. of isocyanuric acid (CA) and
     melamine (M). These aggregates comprise a trismelamine, hub(MIm)3, that
     presents imidazole groups around its periphery; these imidazoles organize
     zinc tetra-Ph porphyrin (ZnTPP) by coordination of the imidazole to the zinc center. Aggregate (1) forms a single rosette upon mixing 1 equiv of
     hub (MIm) 3 and 3 equiv of CA. Adding 3 equiv of ZnTPP yields (2).
     Aggregate (3) forms as a stacked bisrosette upon mixing 2 equiv of
     hub (MIm) 3 and 3 equiv of bisCA. Adding 6 equiv of ZnTPP yields (4).
     stoichiometries of aggregates 1-4 were obtained by titrating the
     trismelamines with CA and by titrating the aggregates with ZnTPP.
     stoichiometry is defined as the ratio at which addnl. CA remains insol. or
     addnl. ZnTPP appears as free ZnTPP in the 1H NMR spectrum. Electrospray
     ionization mass spectrometry (ESI-MS) is compatible with the measured
     stoichiometries. The structures of these aggregates were determined using
     variable-temperature 1H NMR spectroscopy; analogous structures were inferred for
     (5) and (6), the tert-Bu analogs of 1 and 2. The shapes of the traces
     from gel permeation chromatog. (GPC) suggest that imidazole groups
     destabilize the aggregates when they are not involved in coordination to
     zinc; i.e., the stability seems to be 6 \approx 4 > 3 and 5 \approx 2
     > 1. A direct comparison of the relative stability of 1, 2, and 5
     confirms the results of the GPC anal.: mixing 1 (hub (MIm) 3.3CA) with the trismelamine component of 5 (hub (M) 3) gives a 3:2 mixture of 5:1.
     Adding ZnTPP to this solution leads to a 3:2 mixture of 5:2 with free
     trismelamines remaining in solution: 1 is not observed. The results of
     UV/visible spectroscopy are consistent with the other spectroscopic and
     chromatog. results and indicate that 3 equiv of ZnTPP are organized around
     the periphery of 2 and at least 4 equiv around the periphery of 4.
     zinc porphyrinate imidazolyltrismelamine alkylisocyanurate aggregate
     prepn; self assembly prepn zinc porphyrinato aggregate; melamine
     isocyanurate zinc porphyrinate aggregate prepn; porphinate zinc
     imidazolyltrismelamine alkylisocyanurate aggregate prepn
     Complexation kinetics
        (kinetics of complexation of butylimidazole with zinc
        tetraphenylporphyrinato complex)
IT
    Hydrogen bond
        (of aggregates based on rosette of derivs. of isocyanuric acid and
        melamine and their zinc tetraphenylporphyrinato complexes)
IT
     Self-assembly
        (self-assembly preparation of hydrogen-bonded aggregates based on rosette of
        derivs. of isocyanuric acid and melamine and their zinc
        tetraphenylporphyrinato complexes)
     108-77-0, Cyanuric chloride
                                    4422-95-1, 1,3,5-Benzenetricarbonyl chloride midazole 14074-80-7,
     5036-48-6, N-(3-Aminopropyl)imidazole
                                      147355-03-1
     (Tetraphenylporphyrinato)zinc
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (for self-assembly preparation of hydrogen-bonded aggregates based on
        rosette of derivs. of isocyanuric acid and melamine and their zinc
        tetraphenylporphyrinato complexes)
     199171<del>-6</del>3-6P
                                     199171-70-5P
ΙT
                     199171-69-2P
                                                     199171-71-6P
     199171-72-7P 199171-73-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
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(Reactant or reagent)
          (for self-assembly preparation of hydrogen-bonded aggregates based on
          rosette of derivs. of isocyanuric acid and melamine and their zinc
          tetraphenylporphyrinato complexes)
      4316-42-1, N-Butylimidazole
IT
      RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
          (kinetics of complexation of butylimidazole with zinc
          tetraphenylporphyrinato complex)
      199171-74-9P
ΙT
      RL: SPN (Synthetic preparation); PREP (Preparation)
          (preparation of)
      199303-63-4P 199303-64-5P
IT
      RL: SPN (Synthetic preparation); PREP (Preparation)
          (self-assembly preparation of hydrogen-bonded aggregate)
      199171-64-7P 199171-65-8P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
          (self-assembly preparation of hydrogen-bonded aggregate and reaction with
          zinc tetraphenylporphyrinato complex)
      199171-67-0 199171-68-1
      RL: PRP (Properties)
          (stability compared to imidazolyl analog)
                 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE. CNT 16
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(16) Whitesides, G; Acc Chem Res 1995, V27, P37
IT 199171-63-6P 199171-72-7P 199171-73-8P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
          (for self-assembly preparation of hydrogen-bonded aggregates based on
          rosette of derivs. of isocyanuric acid and melamine and their zinc
          tetraphenylporphyrinato complexes)
      199171-63-6 HCAPLUS
      1, 3, 5-Benzenetricarboxamide, N, N', N', -tris[3-[[2-[[4-amino-6-[[3-(1H-imidazol-1-yl)propyl]amino]-1, 3, 5-triazin-2-yl]amino]benzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)
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PAGE 1-B

PAGE 2-A

RN CN

199171-72-7 HCAPLUS
1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-(1, 3-dihydro-1, 3-dioxo-2H-isoindol-2-yl)benzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]-(9CI) (CA INDEX NAME)

PAGE 1-B

PAGE 2-A

199171-73-8 HCAPLUS
1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[(2-aminobenzoyl)][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME) RN CN

PAGE 2-A

199171-64-7P 199171-65-8P IT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(self-assembly preparation of hydrogen-bonded aggregate and reaction with zinc tetraphenylporphyrinato complex)
199171-64-7 HCAPLUS

RN

1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[[3-(1H-imidazol-1-yl)propyl]amino]-1, 3, 5-triazin-2-yl]amino]benzoyl][[4-(1, 1-dimethyl)phenyl]methyl]amino]phenyl]-, compd. with
1-(3, 3-dimethylbutyl)-1, 3, 5-triazin-2, 4, 6(1H, 3H, 5H)-trione (1:3) (9CI) (CA INDEX NAME)

CM 1

CRN 199171-63-6 CMF C108 H114 N30 06

PAGE 1-B

PAGE 2-A

CM 2

CRN 129001-74-7 CMF C9 H15 N3 O3

RN 199171-65-8 HCAPLUS

199171-65-8 HCAPLUS

1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[[3-(1H-imidazol-1-yl)propyl]amino]-1, 3, 5-triazin-2-yl]amino]benzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with

1, 1'-[[4, 6-bis(1-methylethyl)-1, 3-phenylene]bis(methylene)]bis[1, 3, 5-triazine-2, 4, 6(1H, 3H, 5H)-trione] (2:3) (9C1) (CA INDEX NAME)

CM 1

CRN 199171-63-6 CMF C108 H114 N30 06

PAGE 1-A

PAGE 1-B

PAGE 2-A

CM 2

CRN 131296-09-8 CMF C20 H24 N6 O6

199171-67-0 199171-68-1 IT

RL: PRP (Properties)

(stability compared to imidazolyl analog) 199171-67-0 HCAPLUS

RN

1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]benzoyl][[4-(1, 1-dimethylbutyl)phenyl]methyl]amino]phenyl]-, compd. with
1-(3, 3-dimethylbutyl)-1, 3, 5-triazine-2, 4, 6(1H, 3H, 5H)-trione (1:3) (9CI) (CA INDEX NAME)

CM 1

CRN 199171-66-9 CMF C108 H126 N24 06

$$\begin{array}{c} \text{t-Bu} \\ \text{O} \\ \text{NH} \\ \text{NH} \\ \text{CH}2 \\ \text{CH}2 \\ \text{NH} \\ \text{NH} \\ \text{CH}2 \\ \text{CH}2 \\ \text{CH}2 \\ \text{CH}2 \\ \text{CH}2 \\ \text{CH}2 \\ \text{CH}2 \\ \text{NH} \\ \text{Me}_3\text{C-CH}_2 \\ \text{CH}2 \\ \text$$

PAGE 1-B

PAGE 2-A

CM 2

CRN 129001-74-7 CMF C9 H15 N3 O3

RN

199171-68-1 HCAPLUS 1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[(3,3-dimethylbutyl)amino]-1,3,5-triazin-2-yl]amino]benzoyl][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with 1, 1'-[[4,6-bis(1-methylethyl)-1,3-phenylene]bis(methylene)]bis[1,3,5-triazine-2,4,6(1H,3H,5H)-trione] (2:3) (9CI) (CA INDEX NAME) CN

CM

CRN 199171-66-9 CMF C108 H126 N24 06

PAGE 1-A

PAGE 1-B

PAGE 2-A

CM 2

CRN 131296-09-8 CMF C20 H24 N6 06

$$0 \\ \text{H} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{Pr-i}$$

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L51 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
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AN 1997:396315 HCAPLUS

DN 127:122065

ED Entered STN: 26 Jun 1997

TI New polymaleamides from N, N'-ethylenedianilinobisisomaleimide and aromatic diamines by ring-opening polyaddition: synthesis and characterization

AU Nagarajan, E. R.; Rajeswari, N.; Viswanathan, S.

CS Department of Printing Technology, Anna University, Madras, 600 025, India SO Journal of Macromolecular Science, Pure and Applied Chemistry (1997),

SO Journal of Macromolecular Science, Pure and Applied Chemistry (1997), A34(6), 1055-1076

CODEN: ISPCE6; ISSN: 1060-1325

PB Dekker

DT Journal

LA English

CC 35-7 (Chemistry of Synthetic High Polymers)

- AB Polymaleamides have been synthesized by the ring-opening polyaddn. of N,N'-ethylenedianilinobisisomaleimide (EBIMI) with the aromatic diamines, 4,4'-diaminodiphenylmethane, 4,4'-diaminobibenzyl, 4,4'-diaminodiphenyl sulfone, 1,5-diaminonaphthalene, and 2,4-diaminopyridine in 1-methyl-2-pyrrolidinone. The appropriate model compound was also prepared The structures of EBIMI, the model compound, and the polymaleamides were confirmed by IR, UV-visible, 1H NMR spectra, and elemental analyses. The IR spectra revealed the retention of cis-geometry about the C=C bonds in EBIMI and in the polymaleamides. The polymers were characterized by inherent viscosity, solubility, thermal stability, and DSC measurements. The polymaleamides were found to have inherent viscosities in the 0.06-0.13 dL/g range. The polymers were completely soluble in concentrated sulfuric acid and were found to be insol. in organic solvents such as Et alc. and acetone. The thermal degradation behaviors of the polymaleamides were studied by mass spectrometry; proposed fragmentation schemes for the polymaleamides are discussed.
- ST polymaleamide prepn property; ethylenedianilinobisisomaleimide ring opening polym arom diamine

IT Glass transition temperature

(of polymaleamides prepared from N, N'-ethylenedianilinobisisomaleimide and aromatic diamines by ring-opening polyaddn.)

IT Polyamides, preparation

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (polymaleamides from N, N'-ethylenedianilinobisisomaleimide and aromatic diamines by ring-opening polyaddn.)

IT Polymerization

(ring-opening, polyaddn.; of N,N'-ethylenedianilinobisisomaleimide with aromatic diamines)

```
IT
     Polymer degradation
         (thermal; of polymaleamides prepared from N, N'-
         ethylenedianilinobisisomaleimide and aromatic diamines by ring-opening
         polyaddn.)
     174097-15-5P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (intermediate; in preparation of polymaleamides from N, N'-
         ethylenedianilinobisisomaleimide and aromatic diamines by ring-opening
         polyaddn.)
     174097-26-8P
IT
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
         (model compound; in preparation of polymaleamides from N, N'
         ethylenedianilinobisisomaleimide and aromatic diamines by ring-opening
         polyaddn.)
IΤ
     174097-16-6P, N, N'-Ethylenedianilinobisisomaleimide
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (monomer; for preparation of polymaleamides by ring-opening polyaddn.)
     186345-50-6P
                       192508-88-6P
                                         192508-90-0P
                                                          192508-93-3P
IT
     192508-95-5P
                       192508-96-6P
                                         192508-97-7P
                                                          192508-98-8P
                                                                            192508-99-9P
     192588-08-2P
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
         (polymaleamides from N, N'-ethylenedianilinobisisomaleimide and aromatic
         diamines by ring-opening polyaddn.)
                                             108-31-6, 2,5-Furandione, reactions
ΙT
     62-53-3, Benzenamine, reactions
     621-95-4, 4, 4'-Diaminobibenzyl
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reactant; in preparation of polymaleamides from N, N'-
         ethylenedianilinobisisomaleimide and aromatic diamines by ring-opening
         polyaddn.)
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RE. CNT
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RE
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- (48)
- 186345-50-6P
 - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (polymaleamides from N, N'-ethylenedianilinobisisomaleimide and aromatic diamines by ring-opening polyaddn.)
- RN 186345-50-6 HCAPLUS
- Poly[imino(1, 4-dioxo-2-butene-1, 4-diyl) imino-1, 4-phenylenemethylene-1, 4phenyleneimino(1, 4-dioxo-2-butene-1, 4-diyl)imino-1, 4-phenylene-1, 2-ethanediyl-1, 4-phenylene], (Z, Z)- (9CI) (CA INDEX NAME)

PAGE 1-B

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ -\text{CH}_2 & & & \\ \end{array}$$

- ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN L51
- 1997:218626 HCAPLUS
- DN 126:238016
- Entered STN: 04 Apr 1997
- Observation of Diastereomers of the Hydrogen-Bonded Aggregate Hub (M) 3. 3CA Using 1H Nuclear Magnetic Resonance Spectroscopy When CA Is an Optically-Active Isocyanuric Acid
- Simanek, Eric E.; Qiao, Shuang; Choi, Insung S.; Whitesides, George M. AU
- CS Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
 Journal of Organic Chemistry (1997), 62(8), 2619-2621
- S₀
- CODEN: JOCEAH; ISSN: 0022-3263
- American Chemical Society
- DT **Tournal**
- English
- 22-3 (Physical Organic Chemistry)
- The trismelamine component of hub(M)3 contains no chiral centers: the aggregate hub(M)3.3CA exists as a pair of enantiomers in the presence of optically-inactive isocyanuric acid (CA). Optically-active CA-derived from R- or S-naphthylethylamine and phenylethylamine-affords diastereomeric aggregates when mixed with hub (M) 3. These diastereomers are identified using the hydrogen-bonding imide region of the 1H NMR spectrum.
- diastereomer hydrogen bond aggregate proton NMR; isocyanuric acid deriv

```
hydrogen bond aggregate; optically active isocyanuric acid diastereomer
      aggregate
IT
      Molecular association
      Molecular orientation
          (aggregation self-assembly; diastereomers of hydrogen-bonded aggregate
          Hub (M) 3.3CA Using 1H NMR when CA is optically-active isocyanuric
          acid)
      Conformation
      Conformational transition
      Exchange reaction
      Exchange reaction kinetics
      Hydrogen bond
      Inclusion reaction
      Internal rotation
      Optical activity
      Resolution (separation)
      Solvent effect
      Stereoisomerization
      Stereoisomerization kinetics
      Supramolecular structure
          (diastereomers of hydrogen-bonded aggregate Hub (M) 3. 3CA Using 1H
          NMR when CA is optically-active isocyanuric acid)
      Inclusion compounds
      RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
      (Reactant); PROC (Process); RACT (Reactant or reagent)
          (diastereomers of hydrogen-bonded aggregate Hub(M)3.3CA Using 1H
          NMR when CA is optically-active isocyanuric acid)
IT
      NMR (nuclear magnetic resonance)
          (1H; diastereomers of hydrogen-bonded aggregate Hub (M) 3. 3CA
          using 1H NMR when CA is optically-active isocyanuric acid)
      188590-00-3P 188590-01-4P
      RL: PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PRP (Properties); RCT (Reactant); PREP (Preparation); PROC
      (Process); RACT (Reactant or reagent)
          (M (clockwise) and P (counterclockwise) arrangements of complex;
          diastereomers of hydrogen-bonded aggregate Hub (M) 3. 3CA Using 1H
          NMR when CA is optically-active isocyanuric acid)
      188590-02-5P
      RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
          (M (clockwise) and P (counterclockwise) arrangements of complex;
          diastereomers of hydrogen-bonded aggregate Hub (M) 3.3CA Using 1H
          NMR when CA is optically-active isocyanuric acid)
                       188589-98-2
                                         188589-99-3
      188589-78-8
IΤ
      RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
          (diastereomers of hydrogen-bonded aggregate Hub(M)3 3CA Using 1H
          NMR when CA is optically-active isocyanuric acid)
      188589-96-0P
IT
                         188589-97-1P
      RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation);
      RACT (Reactant or reagent)
          (diastereomers of hydrogen-bonded aggregate Hub (M) 3. 3CA Using 1H
          NMR when CA is optically-active isocyanuric acid)
RE. CNT
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RL: PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PRP (Properties); RCT (Reactant); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(M (clockwise) and P (counterclockwise) arrangements of complex; diastereomers of hydrogen-bonded aggregate Hub(M)3.3CA Using 1H NMR when CA is optically-active isocyanuric acid)

RN 188590-00-3 HCAPLUS

1, 3, 5-Benzenetricarboxamide, N, N', N'' -tris[3-[[3-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with (R)-1-[1-(2-naphthalenyl)ethyl]-1,3,5-triazine-2,4,6(1H,3H,5H)-trione (1:3) (9CI) (CA INDEX NAME)

CM 1

CN

CRN 188589-98-2 CMF C15 H13 N3 O3

Absolute stereochemistry. Rotation (+).

CM

CRN 188589-78-8 C108 H123 Br3 N24 06

PAGE 1-A Me3C-CH2-CH2-NH Me3C-CH2-CH2-NH

PAGE 1-B

$$-NH - CH_2 - NH - NH_2 - CH_2 - CH_2 - CMe_3$$

PAGE 2-A

188590-01-4 HCAPLUS RN

1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[3-[[4-amino-6-[(3,3-dimethylbutyl)amino]-1,3,5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with (S)-1-[1-(2-naphthalenyl)ethyl]-1, 3, 5-triazine-2, 4, 6(1H, 3H, 5H)-trione (1:3) (9CI) (CA INDEX NAME) CN

CM 1

CRN 188589-99-3 CMF C15 H13 N3 O3

Absolute stereochemistry. Rotation (-).

CRN 188589-78-8

CMF C108 H123 Br3 N24 06

PAGE 1-B

$$\begin{array}{c} \text{t-Bu} \\ \text{CH}_2 \\ \text{NH} \\ \text{NH} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{NH- CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CMe}_3 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CMe}_3 \\ \text{CH}_2$$

PAGE 2-A

188590-02-5P IT

RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation) (M (clockwise) and P (counterclockwise) arrangements of complex; diastereomers of hydrogen-bonded aggregate Hub (M) 3. 3CA Using 1H NMR when CA is optically-active isocyanuric acid)

188590-02-5 HCAPLUS

188590-02-5 HCAPLUS 1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[3-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with (R)-1-[1-(2-naphthalenyl)ethyl]-1, 3, 5-triazine-2, 4, 6 (1H, 3H, 5H)-trione and (S)-1-[2-(2-naphthalenyl)ethyl]-1, 3, 5-triazine-2, 4, 6 (1H, 3H, 5H)-trione (2:3:3) (9CI) (CA INDEX NAME)

CM 1

CRN 188589-99-3

CMF C15 H13 N3 O3

Absolute stereochemistry. Rotation (-).

CM

188589-98-2 C15 H13 N3 O3 CRN CMF

Absolute stereochemistry. Rotation (+).

CM

CRN 188589-78-8 CMF C108 H123 Br3 N24 O6

PAGE 2-A

188589-78-8 IT

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(diastereomers of hydrogen-bonded aggregate Hub(M)3·3CA Using 1H NMR when CA is optically-active isocyanuric acid)
188589-78-8 HCAPLUS

CN

1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \text{t-Bu} \\ \text{CH}_2 \\ \text{NH} \\ \text{N} \\ \text{NH- CH}_2\text{- CH}_2\text{- CMe}_3 \end{array}$$

PAGE 2-A

L51 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:198079 HCAPLUS

126:238013 DN

Entered STN: 27 Mar 1997 ED

Computations and 1H NMR Spectroscopy of the Imide Region Can Distinguish Isomers of Hydrogen-Bonded Aggregates

ΑU Chin, Donovan N.; Simanek, Eric E.; Li, Xinhua; Wazeer, Mohammed I. M.; Whitesides, George M.

CS Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, ÚSA

S0 Journal of Organic Chemistry (1997), 62(6), 1891-1895 CODEN: JOCEAH; ISSN: 0022-3263

American Chemical Society

DT Journal

English

CC 22-3 (Physical Organic Chemistry)

- General rules for the assignment of isomers of the aggregates of Hub(M)3 (I), a sym. triimide based on a tris(melamine coupled triphenylamine) condensed to a 1, 3, 5-benzenetricarboxylic acid (the Hub) derivative, with cyanuric acid (CA) derivs. using mol. modeling of the I i-Prbenz (CA) 2 and I i-Prfuran (CA) 2 complexes. A simple modification to a noncovalent aggregate can translate into addnl. structural simplicity (due to, in the case of the I complexes, steric repulsion between groups along the periphery of the aggregate). I.e., the use of i-Prbenz (CA) 2 instead of i-Prfuran(CA)2 results in fewer isomers. The rules for interpreting the imide region of the 1H NMR apply to these more complicated aggregates: the suggest the number and symmetries of isomers in solution Aggregates incorporating C3 sym. Hub(M)3 groups are more stable than those that incorporate asym. Hub(M)3 groups. The use of the deviation from planarity (DP) as a computational surrogate for the assignment of relative stability is discussed.
- ST mol modeling hydrogen bonded aggregate isomer; proton NMR imide region aggregate isomer

IT Formation constant

Stability

(deviation from planarity; distinguishment of hydrogen-bonded aggregate isomers by mol. modeling and 1H NMR of imide region)

ΙT Conformation

Conformational transition

Hydrogen bond

Internal rotation

```
Isomers
      Molecular mechanics
      Molecular modeling
      Molecular orientation
      NMR (nuclear magnetic resonance)
      Stereoisomers
      Supramolecular structure
      Symmetry
           (distinguishment of hydrogen-bonded aggregate isomers by mol. modeling
          and 1H NMR of imide region)
IT
      Imides
      Inclusion compounds
      RL: PRP (Properties)
          (distinguishment of hydrogen-bonded aggregate isomers by mol. modeling
          and 1H NMR of imide region)
      Functional groups
           (imide; distinguishment of hydrogen-bonded aggregate isomers by mol.
          modeling and 1H NMR of imide region)
IT
      Molecular association
           (self-assembly; distinguishment of hydrogen-bonded aggregate isomers by
          mol. modeling and 1H NMR of imide region)
0001-74-7 131296-09-8 146651-79-8 1885
IT
                                          146651-79-8 188589-78-8
      RL: RCT (Reactant); RACT (Reactant or reagent)
           (distinguishment of hydrogen-bonded aggregate isomers by mol. modeling
          and 1H NMR of imide region)
      188589-82-4P 188589-86-8P
IT
      RL: SPN (Synthetic preparation); PREP (Preparation)
           (distinguishment of hydrogen-bonded aggregate isomers by mol. modeling
          and 1H NMR of imide region)

13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE. CNT
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      188589-78-8
      RL: RCT (Reactant); RACT (Reactant or reagent)
           (distinguishment of hydrogen-bonded aggregate isomers by mol. modeling
          and 1H NMR of imide region)
      188589-78-8 HCAPLUS
      1, 3, 5-Benzenetricarboxamide, N, N', N', -tris[3-[[3-[[4-amino-6-[(3, 3-
      dimethylbutyl)amino]-1,3,5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)
```

$$\begin{array}{c} \text{t-Bu} \\ \text{CH}_2 \\ \text{NH} \\ \text{NH} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_3 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_3 \\ \text{CH}_2 \\ \text{CH}_3 \\ \text{CH}_3 \\ \text{CH}_3 \\ \text{CH}_4 \\ \text{CH}_2 \\ \text{CH}_3 \\ \text{CH}_3 \\ \text{CH}_4 \\ \text{CH}_5 \\ \text{CH}_5 \\ \text{CH}_5 \\ \text{CH}_5 \\ \text{CH}_6 \\ \text{C$$

PAGE 2-A



IT 188589-82-4P 188589-86-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (distinguishment of hydrogen-bonded aggregate isomers by mol. modeling and 1H NMR of imide region) 188589-82-4 HCAPLUS

RN

1,3,5-Benzenetricarboxamide, N,N',N''-tris[3-[[3-[[4-amino-6-[(3,3-dimethylbutyl)amino]-1,3,5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with 1,1'-[[4,6-bis(1-methylethyl)-1,3-phenylene]bis(methylene)]bis[1,3,5-triazine-2,4,6(1H,3H,5H)-trione] (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 188589-78-8 C108 H123 Br3 N24 06

PAGE 1-B

$$\begin{array}{c} \text{t-Bu} \\ \text{CH}_2 \\ \text{NH} \\ \text{N} \\ \text{NH} \\ \text{CH}_2 - \text{CH}_2 - \text{CMe}_3 \end{array}$$

PAGE 2-A

CM 2

CRN 131296-09-8 CMF C20 H24 N6 06

$$\begin{array}{c} 0 \\ \text{HN} \\ \text{CH}_2 \\ \text{i-Pr} \end{array} \begin{array}{c} 0 \\ \text{CH}_2 \\ \text{Pr-i} \end{array}$$

RN 188589-86-8 HCAPLUS

CN 1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[3-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with 1, 1'-[[3, 4-bis(1-methylethyl)-2, 5-furandiyl]bis(methylene)]bis[1, 3, 5-triazine-2, 4, 6(1H, 3H, 5H)-trione] (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 188589-78-8 CMF C108 H123 Br3 N24 06

PAGE 1-A

PAGE 1-B

$$\begin{array}{c} \text{t-Bu} \\ \text{CH2} \\ \text{NH} \\ \text{CH2} \\ \text{NH-CH2-CH2-CMe3} \end{array}$$

PAGE 2-A

CM 2

CRN 146651-79-8 CMF C18 H22 N6 07

```
L51 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
     1997:71737 HCAPLUS
AN
DN
     126:171999
ED
     Entered STN: 31 Jan 1997
     Synthesis and characterization of new polymaleamides from
     N, N'-bisisomaleimide and N, N'-methylenedianilinobisisomaleimide with some
     aromatic diamines by ring-opening polyaddition
     Viswanathan, S.; Nagarathinam, R.; Rajeswari, N.
AU
     Dep. Polymer Science, Univ. Madras, Madras, 600 025, India
Polymer (1997), 38(1), 217-224
CODEN: POLMAG; ISSN: 0032-3861
CS
S0
PB
     Elsevier
DT
     Journal
LA
     English
     35-7 (Chemistry of Synthetic High Polymers)
CC
     Section cross-reference(s): 27
AR
     Polymaleamides from bisisomaleimides and diamines were prepared by
     ring-opening polyaddn. (ROPA). These polymaleamides were found to have
     inherent viscosity in the range 0.30-0.42 g dl-1. The identities of the
     polymaleamides were confirmed by elemental anal., and IR, UV-visible and
     1H NMR spectroscopies. The thermal degradation behavior of the polymaleamides
     was studied by mass spectrometry and thermogravimetric anal.;
     fragmentation schemes for the polymaleamides are proposed.
     polymaleamide prepn ring opening polyaddn bisisomaleimide; thermal degrdn
     polymaleamide; methylenedianilinobisisomaleimide arom diamine ring opening
     polyaddn
     Polyamides, preparation
     RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
        (maleamide-based; preparation, characterization and thermal degradation of
        polymaleimides prepared by ring-opening polyaddn. of bisisomaleimides)
IT
     Polymerization
         (ring-opening; preparation of polymaleimides by ring-opening polyaddn. of
        bisisomaleimides)
IT
     Polymer degradation
         (thermal; preparation, characterization and thermal degradation of
        polymaleimides prepared by ring-opening polyaddn. of bisisomaleimides)
IT
     62-53-3, Aniline, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (model compound starting material; preparation of bisisomalemide monomers for
        ring-opening polyaddn.)
     57018-29-8P
                   118694-36-3P
     RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
         (model compound; preparation of bisisomalemide monomers for ring-opening
        polyaddn.)
     15189-88-5P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (monomer intermediate; preparation of bisisomalemide monomers for
        ring-opening polyaddn.)
     101-77-9
                                                         302-01-2, Hydrazine,
                 108-31-6, 2,5-Furandione, reactions
     reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (monomer starting material; preparation of bisisomalemide monomers for
        ring-opening polyaddn.)
                                 53024-72-9P
     6330-01-4P
                 6990-21-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
```

```
(monomer; preparation of bisisomalemide monomers for ring-opening polyaddn.)
IT
       5329-22-6P
       RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
       (Reactant or reagent)
            (preparation of bisisomalemide monomers for ring-opening polyaddn.)
                                                186345-47-1P
                                                                       186345-48-2P
IT
       186345-45-9P
                           186345-46-0P
                                                                                            186345-49-3P
                            186345-51-7P
                                                 186345-52-8P
       186345-50-6P
       RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN
       (Synthetic preparation); PREP (Preparation); PROC (Process)
           (preparation, characterization and thermal degradation of)
RE. CNT
                   THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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(30)
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       186345-50-6P
       RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN
       (Synthetic preparation); PREP (Preparation); PROC (Process)
            (preparation, characterization and thermal degradation of)
       186345-50-6 HCAPLUS
CN
       Poly[imino(1, 4-dioxo-2-butene-1, 4-diyl) imino-1, 4-phenylenemethylene-1, 4-
       phenyleneimino(1, 4-dioxo-2-butene-1, 4-diyl)imino-1, 4-phenylene-1, 2-ethanediyl-1, 4-phenylene], (Z, Z)- (9CI) (CA INDEX NAME)
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PAGE 1-B

L51 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:710653 HCAPLUS

DN 126:123234

ED Entered STN: 04 Dec 1996

TI Predicting the Relative Stabilities of Multiparticle Hydrogen-Bonded Aggregates Based on the Number of Hydrogen Bonds and the Number of Particles and Measuring These Stabilities with Titrations Using Dimethyl Sulfoxide

AU Mammen, Mathai; Simanek, Eric E.; Whitesides, George M.

CS Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA

SO Journal of the American Chemical Society (1996), 118(50), 12614-12623 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

CC 68-4 (Phase Equilibriums, Chemical Equilibriums, and Solutions) Section cross-reference(s): 6, 28, 63, 69, 77

AB An exptl. method for determining the relative stabilities of H bonded aggregates in terms of the mol fraction of DMSO in CHCl3 solution (xDMSO) required to cause their dissociation. It also describes 3 indexes (ITm, IG, and IG/(N-1)) that estimate the relative stabilities of H bonded aggregates. Each of these indexes depend on 2 variables, HB and N. HB is the number of H bonds holding the aggregate together; N is the number of particles in the aggregate. The melting-point index (ITm = HB/(N-1)) corresponds conceptually to a "m.p." for the aggregate (i.e., a temperature at which it would dissociate into sep. particles). This index is the most useful of the 3 for "rule of thumb" estimation of relative stability if assembly occurs cooperatively. The free energy index (IG = 2.8HB - 16(N-1)) corresponds to a free energy of assembly (Δ G) with units kcal/mol. The index IG/(N-1) = (2.8HB/(N-1)) - 16 corresponds conceptually to a free energy of association per particle, (Δ G/(N-1)). This 3rd index is most useful if assembly occurs noncooperatively.

ST arom heterocycle hydrogen bonded aggregate stability; NMR DMSO titrn hydrogen bonded aggregate; melamine isocyanuric acid hydrogen bonded

aggregate IT Entropy

Епстору

Free energy Hydrogen bond

Hydrogen bonding enthalpy

Self-association

Stability

(hydrogen-bonded aggregate stability determined by 1H NMR DMSO titration method in CHCl3 solution for aromatic and heterocyclic compds. related to isocyanuric acid and melamine)

IT 141727-14-2

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,

```
nonpreparative)
              (hydrogen-bonded aggregate stability determined by 1H NMR DMSO titration method
             in CHC13 solution for aromatic and heterocyclic compds. related to
             isocyanuric acid and melamine)
        67-68-5, properties
IT
        RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)
              (hydrogen-bonded aggregate stability determined by 1H NMR DMSO titration method
             in CHC13 solution for aromatic and heterocyclic compds. related to
        isocyanuric acid and melamine)
57-44-3 108-78-1D, Melamine, derivs. 108-80
derivs. 129001-73-6 129001-74-7 129001-76-9
                                                                               108-80-5D, Isocyanuric acid,
                               141727-15-3
                                                       146042-01-5
        131296-09-8
                                                                                147355-15-5 154621-58-6
        154621-59-7 154621-61-1
                                                      155786-10-0
                                                                               185943-80-0
                                185943-85-5 185943-88-8
         185943-82-2
                                                                              185943-91-3
        186003-95-2
                                186152-73-8
        RL: PRP (Properties)
              (hydrogen-bonded aggregate stability determined by 1H NMR DMSO titration method
             in CHC13 solution for aromatic and heterocyclic compds. related to
             isocyanuric acid and melamine)
                       THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE. CNT 61
RE
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RL: PRP (Properties)

(hydrogen-bonded aggregate stability determined by 1H NMR DMSO titration method in CHC13 solution for aromatic and heterocyclic compds. related to isocyanuric acid and melamine)

129001-73-6 HCAPLUS

1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

PAGE 3-A

RN

129001-76-9 HCAPLUS
1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with
1-(3, 3-dimethylbutyl)-1, 3, 5-triazine-2, 4, 6(1H, 3H, 5H)-trione (1:3) (9CI) (CA INDEX NAME)

CM 1

CN

CRN 129001-74-7 CMF C9 H15 N3 O3

$$\begin{array}{c} 0 \\ \text{HN} \\ \end{array} \\ \begin{array}{c} \text{CH}_2\text{--}\text{CH}_2\text{--}\text{CMe}_3 \end{array}$$

CM 2

CRN 129001-73-6 CMF C108 H123 Br3 N24 O6

PAGE 2-A

PAGE 3-A

$$\begin{array}{c} & & \\$$

RN

 $\label{eq:continuous} \begin{array}{lll} 154621-58-6 & \text{HCAPLUS} \\ 1, 3, 5-\text{Benzenetricarboxamide}, & \text{N, N', N''-tris}[3-[[2-[[4-amino-6-[[[5-[[[4-amino-6-[[5-[[[4-amino-6-[(3,3-dimethylbutyl)amino]-1,3,5-triazin-2-yl]amino]methyl]-2,4-dimethylphenyl]methyl]amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) & (CA INDEX NAME) \\ \end{array}$ CN

PAGE 1-B

___NH2

PAGE 2-B

$$-\mathsf{CH}_2 \xrightarrow{\mathsf{Me}} \mathsf{CH}_2 - \mathsf{NH} \xrightarrow{\mathsf{N}} \mathsf{NH}_2$$

$$\mathsf{NH} - \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{CMe}_3$$

154621-59-7 HCAPLUS RN

1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[[[5-[[[4-amino-6-[(3,3-dimethylbutyl)amino]-1,3,5-triazin-2-yl]amino]methyl]-2,4-dimethylphenyl]methyl]amino]-1,3,5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with 1,1'-[[4,6-bis(1-methylethyl)-1,3-phenylene]bis(methylene)]bis[1,3,5-triazine-2,4,6(1H,3H,5H)-trione] (1:3) (9CI) (CA INDEX NAME) CN

CM 1

CRN 154621-58-6 CMF C147 H171 Br3 N42 06

PAGE 1-A

-NH₂

PAGE 2-B

$$\begin{array}{c|c} \text{Me} & \text{Me} \\ -\text{CH}_2 - \text{NH} & \text{NH}_2 \\ \hline \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{CMe}_3 \end{array}$$

CM 2

CRN 131296-09-8 CMF C20 H24 N6 06

154621-61-1 HCAPLUS

134021-01-1 HCAPLUS

1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[[[5-[[[4-amino-6-[[3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]methyl]-2, 4-dimethylphenyl]methyl]amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with
1-(3, 3-dimethylbutyl)-1, 3, 5-triazine-2, 4, 6(1H, 3H, 5H)-trione (1:6) (9CI) (CA INDEX NAME) CN

CM 1

CRN 154621-58-6 CMF C147 H171 Br3 N42 06

PAGE 1-A NH-CH2-CH2-CMe3 CH2-NH CH2

PAGE 1-B

PAGE 2-B

$$-\mathsf{CH}_2 \xrightarrow{\mathsf{Me}} \mathsf{CH}_2 - \mathsf{NH} \xrightarrow{\mathsf{N}} \mathsf{NH}_2$$

$$-\mathsf{NH}_2 - \mathsf{CH}_2 - \mathsf$$

CM

CRN 129001-74-7 CMF C9 H15 N3 O3

$$0 \\ \text{HN} \\ \text{CH}_2\text{--} \text{CH}_2\text{--} \text{CMe}_3$$

185943-88-8 HCAPLUS

185943-88-8 HCAPLUS 1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with 1, 1'-[[4, 6-bis(1-methylethyl)-1, 3-phenylene]bis(methylene)]bis[1, 3, 5-triazine-2, 4, 6(1H, 3H, 5H)-trione] (2:3) (9CI) (CA INDEX NAME)

CM

CRN 131296-09-8 CMF C20 H24 N6 O6

CM

CRN 129001-73-6 CMF C108 H123 Br3 N24 06

PAGE 2-A

PAGE 3-A

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ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
     1996:120007 HCAPLUS
AN
DN
     124:177114
ED
     Entered STN: 27 Feb 1996
     Synthesis and characterization of new polymaleamides from
ΤI
     N, N'-ethanedianilinebisisomaleimide with some aromatic diamines
     Nagarajan, E. R.; Rajeswari, N.; Nagarathinam, R.; Viswanathan, S.;
ΑU
     Ramakrishnan, V. T.
Department of Printing Technology, Anna University, Madras, 600 025, India
CS
S<sub>0</sub>
     Polymer International (1996), 39(2), 141-52
     CODEN: PLYIEI; ISSN: 0959-8103
PB
     Wiley
DT
     Journal
     English
LA
CC
     35-5 (Chemistry of Synthetic High Polymers)
AB
     Five polymaleamides were synthesized by the ring-opening polyaddn. of
     N, N'-ethanedianilinebisisomaleimide (EBIMI) with aromatic diamines (having Me
     or methoxy ring substituents) at room temperature; EBIMI was synthesized from
     N, N'-ethanedianilinebismaleamic acid. IR, 13C NMR, and UV-visible
     spectroscopies, inherent viscosity measurements, thermogravimetry,
     differential scanning calorimetry and mass spectrometry were used to
     characterize these polymers.
ST
     ethanedianilinebisisomaleimide prepn copolymn; arom diamine
     ethanedianilinebisisomaleimide copolymn characterization
IT
     Nuclear magnetic resonance
     Polymer degradation
        (of aromatic poly(maleimides) prepared from ethanediyldianilinebisisomaleimi
        de)
IT
     Polyamides, preparation
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
        (preparation and characterization of aromatic poly(maleimides))
IT.
     Chains, chemical
        (structure of aromatic poly(maleimides) prepared from
        ethanediyldianilinebisisomaleimide)
IT
     174097-15-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (intermediate; in preparation of ethanedianilinebisisomaleimide)
     174097-16-6P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
     (monomer; preparation and copolymn. of) 174097-17-7P 174097-18-8P 174097-19-9F
                    174097-18-8P
                                    174097-19-9P
                                                    174097-20-2P
IT
     174097-21-3P
                     174097-22-4P
                                     174097-23-5P
                                                    174097-24-6P
     174097-25-7P
                    174177-87-8P
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
        (preparation and characterization of)
IT
     174097-26-8P
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
```

(preparation and characterization of model compound for polymaleamides) 108-31-6, 2,5-Furandione, reactions 621-95-4, 4,4'-Diaminobibenzyl RL: RCT (Reactant); RACT (Reactant or reagent) IT (starting material; in preparation of ethanedianilinebisisomaleimide)

IT 174097-21-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and characterization of)

RN 174097-21-3 HCAPLUS

Poly[imino[1, 1'-biphenyl]-4, 4'-diylimino(1, 4-dioxo-2-butene-1, 4-diyl) imino-1, 4-phenylene-1, 2-ethanediyl-1, 4-phenyleneimino(1, 4-dioxo-2-butene-1, 4-diyl) (2, 2) (2, 4) (2, 4) (2, 4) (3, 4) (4, 4, 4) (4, 4, 4) (4, 4) (4 diy1)], (Z, Z)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN L51

1996:113713 HCAPLUS

124:202186

Entered STN: 23 Feb 1996 ED

ΤI Synthesis and Evaluation of Thioether-Based Tris-Melamines as Components of Self-Assembled Aggregates Based on the CA M Lattice

Li, Xinhua; Chin, Donovan N.; Whitesides, George M.

Department of Chemistry, Harvard University, Cambridge, MA, 02138, USA CS

S0 Journal of Organic Chemistry (1996), 61(5), 1779-86

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

English

28-20 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 22, 75

Two new tris-melamine derivs., triazine-thio-M3 (M = melamine group-containing ligand) and benzene-thio-M3, were prepared from 2,4,6-trithiocyanuric acid and 1, 3, 5-trimercaptobenzene and a bromobenzyl melamine derivative. In these compds. the central "hub" and the attached "spokes" are attached by thioether linkages rather than amide linkages. These two compds. formed stable and structurally well-defined 1+3 supramol. aggregates with neohexyl isocyanurate as shown by NMR spectroscopy and gel permeation chromatog. 1H NMR competition expts. indicated that the stability of triazine-thio-M3 (neohexyl isocyanurate) 3 was similar to that of benzene-thio-M3 (neohexyl isocyanurate)3. The order of stabilities of tris-melamine-based 1+3 complexes was hubM3 (neohexyl isocyanurate) 3 > triazine-thio-M3 (neohexyl isocyanurate) 3 .apprx. benzene-thio-M3 (neohexyl isocyanurate) 3 > flexM3 (neohexyl isocyanurate) 3. Computational simulations were also carried out on triazine-thio-M3 (neohexyl isocyanurate)3 and hubM3 (neohexyl isocyanurate)3 fully solvated in CHCl3. Values of DP (the deviation from planarity of the cyanuric acid and melamine rosette) obtained from these simulations correlated correctly with the observed stabilities and suggested a structural reason why triazine-thio-M3 (neohexyl isocyanurate) 3 was less stable than

hubM3 (neohexyl isocyanurate) 3.

thioether melamine prepn conformation stability structure; aggregate crystal lattice thioether melamine prepn; crystal structure lattice aggregate melamine thioether; mol structure lattice aggregate melamine thioether

Conformation and Conformers

Crystal structure Molecular structure

Polymer morphology

(preparation and evaluation of thioether-based tris-melamines as components of aggregates)

IT Clusters

Enthalpy and Enthalpy function

Entropy

(preparation and evaluation of thioether-based tris-melamines as components of aggregates based on CA M lattice)

IT Stability

(relative, preparation and evaluation of thioether-based tris-melamines as components of aggregates based on CA·M lattice)

174355-82-9P 174355-90-9P IT

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and evaluation of thioether-based tris-melamines as components of aggregates)

IT 638-16-4, Trithiocyanuric acid 1877-77-6, 3-Aminobenzyl alcohol 15673-00-4 38004-59-0, 1, 3, 5-Trimercaptobenzene 147355-04-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and evaluation of thioether-based tris-melamines as components of aggregates)

174355-83-0P 159217-95-5P 174355-84-1P IT 174355-85-2P 174355-86-3P

174355-87-4P 174355-88-5P 174355-89-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and evaluation of thioether-based tris-melamines as components of aggregates)

174355-82-9P 174355-90-9P IT

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and evaluation of thioether-based tris-melamines as components of aggregates)

174355-82-9 HCAPLUS
Benzamide, N,N',N''-[1,3,5-triazine-2,4,6-triyltris(thiomethylene-3,1-phenylene)]tris[2-[[4-amino-6-[(3,3-dimethylbutyl)amino]-1,3,5-triazin-2-yl]amino]-5-bromo-N-[[4-(1,1-dimethylethyl)phenyl]methyl]- (9CI) (CA CN INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \text{Me}_{3}\text{C}-\text{CH}_{2}-\text{CH}_{2}-\text{NH} \\ \text{H}_{2}\text{N} \\ \text{H}_{2}\text{N} \\ \text{H}_{2} \\ \text{CH}_{2} \\ \text{CH}_{2}-\text{S} \\ \text{N} \\ \text{S}-\text{CH}_{2} \\ \text{CH}_{2} \\ \text{CH}_{4} \\ \text{CH}_{2} \\ \text{CH}_{2} \\ \text{CH}_{3} \\ \text{CH}_{4} \\ \text{CH}_{4} \\ \text{CH}_{4} \\ \text{CH}_{5} \\ \text{CH}_{$$

PAGE 2-A

PAGE 2-B

RN 174355-90-9 HCAPLUS
CN Benzamide, N, N', N''-[1, 3, 5-benzenetriyltris(thiomethylene-3, 1-phenylene)]tris[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromo-N-[[4-(1, 1-dimethylethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

$$-S-CH_2 \longrightarrow N$$

$$H_2N \longrightarrow NH$$

$$Me_3C-CH_2-CH_2-NH$$

PAGE 2-A

- L51 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
- AN 1995:493290 HCAPLUS
- DN 122:264788
- ED Entered STN: 18 Apr 1995
- TI Detection of hydrogen-bonded supramolecular complexes using electrospray ionization from chloroform
- AU Cheng, Xueheng; Gao, Quanyin; Smith, Richard D.; Simanek, Eric E.; Mammen,

Mathia; Whitesides, George M. Chem. Sci. Dep. Environ. Mol. Sci. Lab., Pacific Northwest Lab., Richland, WA, 99352, USA S₀ Rapid Communications in Mass Spectrometry (1995), 9(4), 312-16 CODEN: RCMSEF; ISSN: 0951-4198 Wiley DT Journal LA English CC 22-8 (Physical Organic Chemistry) The stoichiometry of a noncovalent, hydrogen-bonded supramol. complex, AB hub (M) 3. RCA3, was characterized using electrospray ionization from chloroform. The intact (1:3) complex was observed in the neg.-ion mode as a Cl-bound species using Ph4PCl as the source of the charge donor. Collisionally and thermally induced dissociation of the (1:3) complex resulted in the simultaneous loss of all the three RCA units, indicating a cooperative binding of RCA units in the (1:3) complex. These results suggest that the attachment of small, organic-soluble ions may be a useful technique for mass spectrometric characterization of neutral supramol. complexes that are stable or soluble only in nonpolar organic solvents. ST hydrogen bonded supramol complex mass spectra; supramol complex electrospray ionization mass spectra Hydrogen bond IT Mass spectra (detection of hydrogen-bonded supramol. complexes using electrospray ionization from chloroform) 2001-45-8, Tetraphenylphosphonium chloride RL: NUU (Other use, unclassified); USES (Uses) (detection of hydrogen-bonded supramol. complexes using electrospray ionization from chloroform) 129001-76-9 RL: PRP (Properties) (detection of hydrogen-bonded supramol. complexes using electrospray ionization from chloroform) IT 129001-76-9 RL: PRP (Properties) (detection of hydrogen-bonded supramol. complexes using electrospray ionization from chloroform) 129001-76-9 HCAPLUS 1, 3, 5-Benzenetricarboxamide, N, N', N', -tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-1, 3, 3-triazin-2-yl]amino]-1, 3-triazin-2-yl]amino[-1, 3-triazin-2-yl]amino[-1, 3-triazin-2-yl]amino[dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with 1-(3, 3-dimethylbutyl)-1, 3, 5-triazine-2, 4, 6(1H, 3H, 5H)-trione (1:3) (9CI) (CA INDEX NAME) CM CRN 129001-74-7 CMF C9 H15 N3 O3

CH2-CH2-CMe3

CM

CRN 129001-73-6 CMF C108 H123 Br3 N24 06

$$\begin{array}{c} \text{NH-CH}_2\text{-CH}_2\text{-CMe}_3 \\ \text{NH-CH}_2\text{-CH}_2\text{-CMe}_3 \\ \text{NH-CH}_2\text{-CH}_2\text{-CMe}_3 \\ \text{H}_2\text{N} \\ \text{NH-CH}_2\text{-CH}_2\text{-CMe}_3 \\ \text{t-Bu} \end{array}$$

PAGE 2-A

PAGE 3-A

- ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN 1994: $456892\,$ HCAPLUS L51
- AN
- 121:56892 DN
- Entered STN: 06 Aug 1994 ED
- Self-Assembly through Hydrogen Bonding: Preparation and Characterization of Three New Types of Supramolecular Aggregates Based on Parallel Cyclic CA3·M3 "Rosettes"
 Mathias, John P.; Seto, Christopher T.; Simanek, Eric E.; Whitesides, ΤI
- ΑÜ

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George M.
     Department of Chemistry, Harvard University, Cambridge, MA, 02138, USA Journal of the American Chemical Society (1994), 116(5), 1725-36
SO
     CODEN: JACSAT; ISSN: 0002-7863
DT
     Journal
     English
LA
\alpha
     22-13 (Physical Organic Chemistry)
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
     Reaction of hub (MM) 3, a compound (I) containing six melamines, with monomeric,
     dimeric, and trimeric derivs. of isocyanuric acid yields three new types
     of hydrogen-bonded self-assembled supramol. aggregates. These new
     aggregates are represented by hub (MM) 3:3benz (CA) 2 and
     hub (MM) 3:3furan (CA) 2, hub (MM) 3:6neohex (CA), and
     hub (MM) 3:3neohex (CA):C18hub (CA) 3 [e.g., benz (CA) 2 = II]. These supramol.
     aggregates are composed of 4-7 individual mols. and have mol. wts. in the
     range 4.1-6.3 kDa. Each aggregate is stabilized by 36 hydrogen bonds in two parallel cyclic CA3 M3 "rosettes". Characterization of these
     aggregates by 1H and 13C NMR spectroscopies, gel permeation chromatog.,
     and vapor pressure osmometry confirms that each exists as a stable, well-defined structure in chloroform or methylene chloride solns. The
     design of these self-assembled aggregates, their relative stabilities, and
     the techniques used for their characterization are discussed. The
     operation of pos. cooperativity in the self-assembly of hub (MM) 3:6 neohex (CA) is demonstrated. The self-assembly of
     hub (MM) 3: 3 neohex (CA): C18 hub (CA) 3 demonstrates the controlled aggregation
     of three different components into a single supramol. aggregate. The size
     and stability of these self-assembled aggregates are correlated with
     results obtained from gel permeation chromatog.
     self assembly hydrogen bond; supramol aggregate rosette; melamine hydrogen
     bond isocyanuric acid
IT
     Hydrogen bond
     Molecular association
         (hydrogen-bonded self-assembled supramol. aggregates of melamine
         derivs. with isocyanuric acid derivs.)
     1333-74-0
IT
     RL: PRP (Properties)
         (hydrogen bond, hydrogen-bonded self-assembled supramol. aggregates of
         melamine derivs. with isocyanuric acid derivs.)
19-05-0P 32280-53-8P 154621-52-0P 154621-53-1P
     1889-05-0P
                                                                       154621-54-2P
     154621-55-3P
                      154621-56-4P
                                       154621-57-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (intermediate in preparation of precursor for hydrogen-bonded self-assembled
         supramol. aggregates)
IT
     154621-58-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation and participation in hydrogen-bonded self-assembled supramol.
         aggregates with isocyanuric acid derivs.)
     154621-59-7P 154621-60-0P 154621-61-1P 154621-62-2P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
     108-38-3, m-Xylene, reactions 108-77-0, Cyanuric chloride
                                                                             4422-95-1.
      1, 3, 5-Benzenetricarbonyl trichloride 58632-95-4
                                                                147355-07-5
     RL: PRP (Properties)
         (reactant, in preparation of precursor for hydrogen-bonded self-assembled
         supramol. aggregates)
     154621-58-6P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation and participation in hydrogen-bonded self-assembled supramol.
         aggregates with isocyanuric acid derivs.)
     154621-58-6 HCAPLUS
RN
     1, 3, 5-Benzenetricarboxamide, N, N', N'-tris[3-[[2-[[4-amino-6-[[5-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]methyl]-2, 4-
CN
```

dimethylphenyl]methyl]amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-

(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

___NH2

PAGE 2-B

$$-\mathsf{CH}_2 \xrightarrow{\mathsf{Me}} \mathsf{CH}_2 - \mathsf{NH} \xrightarrow{\mathsf{N}} \mathsf{NH}_2$$

$$\mathsf{NH} - \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{CMe}_3$$

154621-59-7P 154621-60-0P 154621-61-1P 154621-62-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

154621-59-7 HCAPLUS

1, 3, 5-Benzenetricarboxamide, N, N', N' -tris[3-[[2-[[4-amino-6-[[[5-[[[4-amino-6-[(3,3-dimethylbutyl)amino]-1,3,5-triazin-2-yl]amino]methyl]-2,4-dimethylphenyl]methyl]amino]-1,3,5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with 1,1'-[[4,6-bis(1-methylethyl)-1,3-phenylene]bis(methylene)]bis[1,3,5-triazine-2,4,6(1H,3H,5H)-trione] (1:3) (9CI) (CA INDEX NAME)

CM

154621-58-6 CRN CMF C147 H171 Br3 N42 06

PAGE 1-A NH-CH2-CH2-CMe3 NH-CH2-Me t-Bu

-NH2

PAGE 2-B

$$\begin{array}{c} \text{Me} \\ -\text{CH}_2 \\ \text{CH}_2 - \text{NH} \\ \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{CMe}_3 \end{array}$$

$$- \text{CH}_2 - \text{NH} - \text{NH}_2$$

$$- \text{Me}$$

$$- \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{CMe}_3$$

CM 2

CRN 131296-09-8 CMF C20 H24 N6 06

$$\begin{array}{c|c} O & O & O \\ \hline \\ I - Pr & Pr - i \end{array}$$

154621-60-0 HCAPLUS

154621-60-0 HCAPLOS

1, 3, 5-Benzenetricarboxamide, N, N', N'-tris[3-[[2-[[4-amino-6-[[[5-[[[4-amino-6-[[3,3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]methyl]-2, 4-dimethylphenyl]methyl]amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with

1, 1'-[[3, 4-bis(1-methylethyl)-2, 5-furandiyl]bis(methylene)]bis[1, 3, 5-triazine-2, 4, 6(1H, 3H, 5H)-trione] (1:3) (9CI) (CA INDEX NAME) CN

CM 1

CRN 154621-58-6 CMF C147 H171 Br3 N42 06

PAGE 1-A NH-CH2-CH2-CMe3 NH-CH2

PAGE 1-B

PAGE 2-B

$$-\mathsf{CH}_2 - \mathsf{NH} - \mathsf{NH}_2 \\ -\mathsf{NH} - \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{CH}_2 \\$$

CM 2

CRN 146651-79-8 CMF C18 H22 N6 07

$$0 \\ \text{H} \\ \text{CH}_2 \\ \text{O} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{NH}$$

154621-61-1 HCAPLUS

1,3,5-Benzenetricarboxamide, N,N',N''-tris[3-[[2-[[4-amino-6-[[[5-[[[4-amino-6-[(3,3-dimethylbuty])amino]-1,3,5-triazin-2-yl]amino]methyl]-2,4-dimethylphenyl]methyl]amino]-1,3,5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with
1-(3,3-dimethylbutyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione (1:6) (9CI) (CA INDEX NAME)

CM 1

CRN 154621-58-6 CMF C147 H171 Br3 N42 06 ·

PAGE 1-B

 $-NH_2$

PAGE 2-B

$$\begin{array}{c} \text{Me} \\ -\text{CH}_2 \\ -\text{CH}_2 - \text{NH} \\ -\text{NH}_2 \\ -\text{NH}_2 \\ -\text{CH}_2 - \text{CH}_2 - \text{CMe}_3 \end{array}$$

CM 2

CRN 129001-74-7 CMF C9 H15 N3 O3

$$\begin{array}{c} \text{O} \\ \text{H} \\ \text{CH}_2\text{--} \\ \text{CH}_2\text{--} \\ \text{CHe}_3 \\ \end{array}$$

RN 154621-62-2 HCAPLUS

1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[[[5-[[[4-amino-6-[([5-[[[4-amino-6-[([5-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]methyl]-2, 4-dimethylphenyl]methyl]amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with N, N', N''-tris[2-[octadecyl[5-(octadecyloxy)-2-(tetrahydro-2, 4, 6-trioxo-1, 3, 5-triazin-1(2H)-yl)benzoyl]amino]phenyl]-1, 3, 5-benzenetricarboxamide (1:3) (9CI) (CA INDEX NAME)

CM 1

CRN 154621-58-6 CMF C147 H171 Br3 N42 06

PAGE 1-B

-NH₂

PAGE 2-B

$$-\mathsf{CH}_2 \xrightarrow{\mathsf{Me}} \mathsf{CH}_2 - \mathsf{NH} \xrightarrow{\mathsf{N}} \mathsf{NH}_2$$

$$\mathsf{NH} - \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{CMe}_3$$

$$-\mathsf{CH}_2-\mathsf{NH}-\mathsf{NH}_2\\ -\mathsf{Me}\\ \mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CMe}_3$$

CM 2

CRN 146042-01-5 CMF C165 H255 N15 018

PAGE 1-A

```
L51 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
     1994:322644 HCAPLUS
AN
DN
     120:322644
ED
     Entered STN: 25 Jun 1994
     Self-assembly through hydrogen bonding: structures based on cyanuric
     acid. melamine
     Mathias, John P.; Seto, Christopher T.; Whitesides, George M.
     Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA
     Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1993), 34(1), 92-3
     CODEN: ACPPAY; ISSN: 0032-3934
DT
     Journal
LA
     English
CC
     22-13 (Physical Organic Chemistry)
```

The self-assembly of melamine derivs., e.g. I (only one substituent shown), with cyanuric acid derivs., e.g. II, occurred through hydrogen bonding, e.g. in I.3II. ST self assembly hydrogen bonding; cyanuric acid melamine self assembly; supramol aggregate hub spoke arrangement IT Hydrogen bond Molecular association (of melamine derivs. with cyanuric acid derivs. in supramol. structures) ΙT 1333-74-0 RL: PRP (Properties) (hydrogen bond, of melamine derivs. with cyanuric acid derivs. in supramol. structures) 129001-73-6 154621-58-6 RL: PRP (Properties) (hydrogen bonding of, with cyanuric acid derivs.) IT 129001-74-7, 1, 3, 5-Triazine-2, 4, 6(1H, 3H, 5H)-trione, 1-3, 3-dimethylbutyl)-RL: PRP (Properties) (hydrogen bonding of, with melamine derivs.) 129001-73-6 154621-58-6 ΙT RL: PRP (Properties) (hydrogen bonding of, with cyanuric acid derivs.) 129001-73-6 HCAPLUS 1, 3, 5-Benzenetricarboxamide, N, N', N', -tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino] dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

PAGE 3-A

RN CN

 $154621-58-6 \quad HCAPLUS \\ 1, 3, 5-Benzenetricarboxamide, \quad N, N', N''-tris[3-[[2-[[4-amino-6-[[[5-[[4-amino-6-[(3,3-dimethylbutyl)amino]-1,3,5-triazin-2-yl]amino]methyl]-2, 4-dimethylphenyl]methyl]amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)$

PAGE 1-B

 $-NH_2$

$$\begin{array}{c} \text{Me} \\ -\text{CH}_2 \\ \text{CH}_2 - \text{NH} \\ \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{CMe}_3 \end{array}$$

```
L51 ANSWER 13 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
     1993:604476 HCAPLUS
AN
     119:204476
DN
ED
     Entered STN: 13 Nov 1993
ΤI
     Cure optimization studies of polyamino bis-itaconimide polymer by TMA and
AII
     Krishnan, K.; Vijayan, T. M.; Ninan, K. N.
     Propellants Spec. Chem. Group, Vikram Sarabhai Space Cent., Trivandrum,
     695022, India
S0
     Proc. Natl. Symp. Therm. Anal., 8th (1991), 385-7. Editor(s): Dharwadkar,
     S. R. Publisher: Indian Therm. Anal. Soc., Bombay, India. CODEN: 58QBAY
DT
     Conference
LA
     English
     37-5 (Plastics Manufacture and Processing)
N, N'-bis(itaconamic acid) p, p'-diphenylmethane, prepared by reacting itaconic anhydride and p, p'-diaminodiphenylmethane, was chemical imidized in
     DMF. The chain extended polyaminobisitaconimide polymer was prepared by
     Michael type addition reaction of the pre-polymer and the same aromatic diamine.
     The resin cured under pressure was evaluated for its glass transition
     temperature, thermal stability, and degradation kinetics using thermoanal.
     techniques such as thermomech. anal. and thermogravimetry. The effect of post-cure on the thermal behavior of the polymer was studied in detail.
ST
     cure optimization polyaminobisitaconimide thermal analysis; itaconimide
     polymer cure optimization
     Polyimides, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (bisitaconimide-based, crosslinking of, optimization of, thermal anal.
         for)
ΙT
     Glass temperature and transition
         (of bis(itaconamic acid) polyimides)
     Crosslinking
ΙT
         (of bis(itaconamic acid) polyimides, optimization of, thermal anal. of)
     102773-39-7
                     102792-51-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (crosslinking of, optimization of, thermal anal. for)
1T
     102773-39-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (crosslinking of, optimization of, thermal anal. for)
     102773-39-7 HCAPLUS
     Poly[imino(2-methylene-1, 4-dioxo-1, 4-butanediyl)imino-1, 4-
     phenylenemethylene-1, 4-phenyleneimino (3-methylene-1, 4-dioxo-1, 4-
     butanediyl)imino-1,4-phenylenemethylene-1,4-phenylene] (9CI) (CA INDEX
```

PAGE 1-B

```
L51 ANSWER 14 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
     1993:254892 HCAPLUS
AN
DN
     118:254892
ED
     Entered STN: 26 Jun 1993
ΤI
     Molecular self-assembly through hydrogen bonding: supramolecular
     aggregates based on the cyanuric acid-melamine lattice
IIA
     Seto, Christopher T.; Whitesides, George M.
     Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA
Journal of the American Chemical Society (1993), 115(3), 905-16
S<sub>0</sub>
     CODEN: JACSAT; ISSN: 0002-7863
DT
     Journal
     English
     28-23 (Heterocyclic Compounds (More Than One Hetero Atom))
CC
     Section cross-reference(s): 1
0S
     CASREACT 118:254892
AB
     Reaction of the tris(melamine) derivs. hubM3 (C6H3-1, 3, 5-[CONHC6H4-3-
     N(CH2C6H4-4-CMe3)COC6H3-2-NHC3N3(NH2)(NHCH2CH2CMe3)-5-Br]3) and
      flexM3 (C6H3-1, 3, 5-[CO2 (CH2) 30COC6H4-2-NHC3N3 (NH2) (NHCH2CH2CMe3)] 3) \ with \\
     RICA (neohexyl isocyanurate) and R2CA (3, 3, 3-triphenylpropyl isocyanurate), resp., in CHCl3 yields structurally well-defined supramol. aggregates hubM3(R1CA)3 and flexM3(R2CA)3. These structures were characterized using 1H NMR, 13C NMR, and UV spectroscopy, gel permeation
     chromatog., and vapor pressure osmometry. FlexM3 is a conformationally
     flexible analog of hubM3. The greater degree of preorganization that is
     build into the mol. structure of hubM3 compared to flexM3 makes
     hubM3(R1CA)3 a more stable aggregate than flexM3(R2CA)3. These
     self-assembling structures are the first step in a program to design,
     synthesize, and develop methods to characterize supramol. complexes that
     are held together by networks of noncovalent interactions.
ST
     supramol aggregate cyanuric acid melamine lattice; RNA supramol aggregate
     cyanuric acid melamine; safety use nitro compd
IT
     Hydrogen bond
         (in cyanuric acid-melamine supramol. aggregates)
IT
     Safety
         (in handling nitro compds.)
IT
     900-91-4, 3, 3, 3-Triphenylpropanoic acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (chlorination of)
IT
     541-69-5
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (dimethylethoxycarbonylation of)
     1333-74-0
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (hydrogen bond, in cyanuric acid-melamine supramol. aggregates)
IT
     108-19-0, Biuret
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (nitration of)
ΙT
     147355-04-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
```

```
(Reactant or reagent)
        (preparation and chlorination of)
ΙT
     68621-88-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and condensation reaction of, with tert-butylbenzyl bromide)
     129001-76-9P
                   147860-68-2P
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
        (preparation and properties of)
     147355-09-7P
                   147355-10-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with benzenetricarbonyl chloride)
     147355-03-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with bromobenzoyl chloride)
    88-95-9P, Phthaloyl dichloride 147355-06-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with cyanuric chloride)
     147355-14-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with di-Et carbonate)
     147355-05-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with hydrazine)
     129001-73-6P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with neohexyl isocyanurate)
    147355-07-5P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with neohexylamine)
    94964-61-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with nitrobiuret)
     147355-08-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with trifluoroacetic acid)
     147355-12-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with triphenylpropyl isocyanurate)
     129001-74-7P 147355-15-5P
ΙT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with tris(melamine) derivative)
IT
     147355-11-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction with di-Et carbonate)
IT
    16326-62-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction with dimethylbutylamine)
ΙT
     147355-13-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reduction of)
ΙT
     41839-95-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     18880-00-7
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
```

```
(reaction of, with [(dimethylethoxy)carbonyl]diaminobenzene)
             504-63-2, 1,3-Propanediol RL: RCT (Reactant); RACT (Reactant or reagent)
IT
                       (reaction of, with anthranilic acid)
             108-77-0, Cyanuric chloride
IT
             RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with carbamate derivative)
             58632-95-4
             RL: RCT (Reactant); RACT (Reactant or reagent)
                       (reaction of, with diaminobenzene)
IT
             5794-88-7
             RL: RCT (Reactant); RACT (Reactant or reagent)
                       (reaction of, with phthaloyl dichloride)
             118-92-3, Anthranilic acid
             RL: RCT (Reactant); RACT (Reactant or reagent)
             (reaction of, with propanediol) 4422-95-1, 1,3,5-Benzenetricarbonyl trichloride
             RL: RCT (Reactant); RACT (Reactant or reagent)
                       (reaction of, with triazinyl aminophenylamine derivative)
IT
             15673-00-4
             RL: RCT (Reactant); RACT (Reactant or reagent)
                       (reactions of, with nitrobiuret or carbamate derivative)
IT
             15207-30-4
             RL: RCT (Reactant); RACT (Reactant or reagent)
                       (tert-butoxycarbonylation of)
IT
             129001-76-9P
             RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
                       (preparation and properties of)
              129001-76-9 HCAPLUS
             1, 3, 5-Benzenetricarboxamide, N, N', N', -tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-1, 3, 5-triazin-2-yl]amino[-1, 3, 5-triazin-2-yl]amino[-1, 3, 5-triazin-2-
CN
             dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with 1-(3, 3-dimethylbutyl)-1, 3, 5-triazine-2, 4, 6(1H, 3H, 5H)-trione (1:3) (9CI)
              (CA INDEX NAME)
             CM
                          1
             CRN 129001-74-7
             CMF C9 H15 N3 O3
                               CH2-CH2-CMe3
             CM
```

CRN 129001-73-6

CMF C108 H123 Br3 N24 O6

$$\begin{array}{c} \text{NH-CH}_2\text{-CH}_2\text{-CMe}_3 \\ \text{NH-CH}_2\text{-CMe}_3 $

PAGE 2-A

PAGE 3-A

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IT

129001-73-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with neohexyl isocyanurate)

RN CN

129001-73-6 HCAPLUS

1, 3, 5-Benzenetricarboxamide, N, N', N' -tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

PAGE 3-A

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- L51 ANSWER 15 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1991:41995 HCAPLUS
- DN 114:41995
- ED TI
- Entered STN: 09 Feb 1991
 Self-assembly of a hydrogen-bonded 2 + 3 supramolecular complex Seto, Christopher T.; Whitesides, George M.
 Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA
 Journal of the American Chemical Society (1991), 113(2), 712-13
- ΑU
- CS S0

```
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 22-13 (Physical Organic Chemistry)
GI
```

$$0 \xrightarrow{\text{HN}} 0 \xrightarrow{\text{Me}_2\text{CH}} \xrightarrow{\text{CHMe}_2} 0 \xrightarrow{\text{NH}} 0$$

Reaction of the tris(melamine) C6H3-1, 3, 5-[CONHC6H4-3-N(CH2C6H4-4-C(CH3)3)COC6H3-2-NHC3N3(NH2)(NHCH2CH2C(CH3)3)-5-Br]3 (hubM3) with the bis (cyanuric acid) I in CHC13 or CH2C12 yields a complex (hubM3)2(I)3. The formation of this complex illustrates the use of mol. self-assembly to form a large (in this instance, MW 5519) complex structure with defined 3-dimensional shape held together through networks of H bonds. supramol hydrogen bonded complex; melamine cyanuric acid complex; mol self assembly hydrogen bonded complex; Overhauser effect hydrogen bonded complex IT Overhauser effect (in hydrogen-bonded bis(cyanuric acid)-tris(melamine) supramol. complex) IT Hydrogen bond (of bis(cyanuric acid) with tris(melamine) in self-assembled supramol. complex) IT 1333-74-0 RL: PRP (Properties) (hydrogen bond, of bis(cyanuric acid) with tris(melamine) in self-assembled supramol. complex) 129001-73-6 RL: PRP (Properties) IT (hydrogen bonding of, with bis(cyanuric acid) derivative in self-assembled supramol. complex) 131296-09-8 RL: PRP (Properties) (hydrogen bonding of, with tris(melamine) in self-assembled supramol. complex)

IT 129001-73-6
RI: PRP (Prov

RL: PRP (Properties)
(hydrogen bonding of, with bis(cyanuric acid) derivative in self-assembled supramol. complex)

RN 129001-73-6 HCAPLUS

1, 3, 5-Benzenetricarboxamide, N, N', -tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

PAGE 3-A

$$\begin{array}{c} & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

- ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN 1990:532138 HCAPLUS L51
- AN
- DN 113:132138
- ED
- TI
- AU
- CS S0
- Entered STN: 13 Oct 1990
 Self-assembly based on the cyanuric acid-melamine lattice
 Seto, Christopher T.; Whitesides, George M.
 Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA
 Journal of the American Chemical Society (1990), 112(17), 6409-11

```
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 113:132138
```

```
Reaction of the tris(melamine) derivative 1, 3, 5-R3C6H3 (R = Q) with N-neohexyl
AB
               cyanurate in CHCl3 or CH2Cl2 gave a soluble derivative of the planar lattice of
               the 1:1 complex of melamine and cyanuric acid.
               neohexyl cyanurate complexation trismelamine; melamine tris complexation
               neohexyl cyanurate; cyanuric acid melamine complex structure
               Molecular structure
                         (of melamine-cyanuric acid complex)
IT
               129001-73-6
               RL: RCT (Reactant); RACT (Reactant or reagent)
                         (complexation of, with neohexyl cyanurate)
IT
               129001-74-7
               RL: RCT (Reactant); RACT (Reactant or reagent)
                         (complexation of, with tris(melamine) derivative)
               129001-76-9P
IT
               RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
                         (preparation and mol. structure of)
               129001-73-6
RL: RCT (Reactant); RACT (Reactant or reagent)
                         (complexation of, with neohexyl cyanurate)
               129001-73-6 HCAPLUS
RN
               1, 3, 5-Benzenetricarboxamide, N, N', N''-tris[3-[[2-[[4-amino-6-[(3, 3-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1, 1-dimethylbutyl)amino]-1, 3, 5-triazin-2-yl]amino]-1,             dimethylethyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)
```

PAGE 2-A

PAGE 3-A

$$\begin{array}{c} & & \\$$

IT

129001-76-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and mol. structure of)
129001-76-9 HCAPLUS

RN CN 1,3,5-Benzenetricarboxamide, N,N',N''-tris[3-[[2-[[4-amino-6-[(3,3-dimethylbutyl)amino]-1,3,5-triazin-2-yl]amino]-5-bromobenzoyl][[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, compd. with 1-(3,3-dimethylbutyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione (1:3) (9CI) (CA INDEX NAME) CM 1

CRN 129001-74-7 CMF C9 H15 N3 O3

$$\begin{array}{c} 0 \\ \text{H} \\ \end{array} \\ \begin{array}{c} \text{CH}_2\text{--} \\ \text{CH}_2\text{---} \\ \text{CH}_2\text{---} \\ \text{CMe}_3 \end{array}$$

CM 2

CRN 129001-73-6 CMF C108 H123 Br3 N24 06

PAGE 1-A

PAGE 2-A

PAGE 3-A

```
ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
     1986:425024 HCAPLUS
AN
DN
     105:25024
     Entered STN: 26 Jul 1986
ED
     Development of bis(itaconimide)s for composites
TI
     Vijayan, T. M.; Bisht, Singh; Rao, K. V. C.
AU
     Polym. Spec. Chem. Div., Vikram Sarabhai Space Cent., Trivandrum, 695022,
CS
     Journal of Polymer Materials (1985), 2(2), 81-7
S0
     CODEN: JOPME8; ISSN: 0970-0838
     Journal
DT
     English
CC
     37-3 (Plastics Manufacture and Processing)
     The preimidized precursor polyimide based on itaconic anhydride (I)
     [2170-03-8] and p, p'-diaminodiphenylmethane (II) [101-77-9] was developed
     as a resin matrix for glass fiber composites. The monomer
     N, N'-bis(itaconamic acid)-p, p'-diphenylmethane [66461-25-4] was prepared by treating I with II in Me2CO. The imidization and prepolymer synthesis was carried out in DMF. The polymer [102792-52-9] without chain extender showed less flexural properties because of the high crosslink d. of the
     cured polybisitaconimide. The incorporation of II reduced the crosslink
     d. of polybisitaconimide and thus increased flexural properties of the
     laminates.
ST
     itaconic anhydride reaction aminodiphenylmethane; polyimide
     diaminodiphenylmethanebisitaconamic acid; aminodiphenylmethane copolymer
     diaminodiphenylmethanebisitaconamic acid; glass fiber reinforced polyimide
     bisitaconimide
     Glass fibers, uses and miscellaneous
     RL: USES (Uses)
         ([bis(itaconamic acid)]diphenylmethane polyimide reinforced with, with
         good flexural properties)
     Polyimides, preparation
     RL: SPN (Synthetic preparation); PREP (Preparation)
         ([bis(itaconamic acid)]diphenylmethane, preparation and properties of)
IT
     102792-52-9
     RL: USES (Uses)
     (glass fiber-reinforced)
102773-39-7 102792-51-8
ΙT
     RL: USES (Uses)
          (glass fiber-reinforced, with good flexural properties)
     66461-25-4P
IT
     RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
         (preparation and polymerization of)
IT
     2170-03-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
          (reaction of, with diaminodiphenylmethane)
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
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butanediyl)imino-1, 4-phenylenemethylene-1, 4-phenylene] (9CI) (CA INDEX

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NAME)

65:38104

OREF 65:7051d-h, 7052a-f Entered STN: 22 Apr 2001 ED Reaction of malonamide derivatives under conditions of the Mannich ΤI reaction AU Braeuniger, H.; Stens, B. Univ. Rostock, Germany Pharmazie (1963), 18(9), 585-600 SO CODEN: PHARAT; ISSN: 0031-7144 DT Journal German CC 33 (Aliphatic Compounds) For diagram(s), see printed CA Issue. GΙ A series of malonamides with substituents on the amide groups or on the C-2 atom were examined under a variety of exptl. conditions for Mannich condensation. The observed lack of reaction, isolation of a bis-substituted methylene compound, or formation of the Mannich base is discussed in terms of the relative nucleophilicity of the C-2 atom on the malonamide compound Malondiamide (I), m. 170° , was obtained in 85% yield from 50 g. diethyl malonate (II) and 150 ml. 25% aqueous ammonium hydroxide, after standing at room temperature for 2 hrs. Dropwise addition of 0.01 mole methylenebispiperidine (III) to 0.02 mole I in EtOH, followed by 12 hrs. at reflux, afforded 27% methylenebismalondiamide (IV), m. 274°. In all attempts to condense I under Mannich conditions with 35% aqueous H2CO and morpholine, I was recovered unchanged. With piperidine, or secondary aliphatic amines as the free bases or their HCl salts, I gave IV but no Mannich base. Finely powdered I (5.01 g.) in 25 ml. MeOH and 50 ml. 2N sodium methoxide was treated with 15 ml. MeI to yield 36% methylmalondiamide (V), m. 212-15°. Similarly, I with EtI and NaOEt gave 39% EtCH(CONH2)2 (VI), m. 218°; with CH2:CHCH2Br and NaOBu, I gave 7% CH2:CHCH2CH(CONH2)2 (VII), m. 206-7°; and with Phl and NaOEt, I gave 20% PhCH(CO NH2)2 (VIII), m. 210-12°. Attempts to condense V with morpholine gave no reaction, but under Mannich conditions with morpholine hydrochloride, piperidine, Bu2NH, iso-Bu2NH, Pr2NH, and iso-Pr2NH as either the free bases or the HCl salts, V gave 30-45% CH2[CMe(CONH2)2]2, m. 224-35°. VII (1.4 g.) in excess H2CO solution was treated dropwise with an equivalent amount of piperidine to yield

. apprx. 8% of the Mannich base, piperidinomethylallylmalondiamide, m. 144°. Similarly, with iso-Bu2NH was obtained apprx.10% diisobutylaminomethylallylmalondiamide, m. 109°. II (12.8 g.) and 21.6 g. benzylamine was refluxed 2 hrs. on a sand bath. Material boiling below 160° was removed by distillation to afford as residue 71% CH2 (CONHCH2Ph) 3 (IX), m. 141° (EtOH). Similarly, 12.8 g. II with 20 g. cyclohexylamine gave 32% malondicyclohexylamide (X), m. 162-5°; II (16 g.) with 174.2 g. morpholine at reflux for 20 hrs. gave 78% malondimorpholine (XI), m. 136° (EtOH). Upon treatment with III, as for I, IX formed 43% methylenebis (malondibenzylamide) (XII), m. 244°. Mannich conditions using IX, H2CO, and morpholine hydrochloride, piperidine, or secondary aliphatic amines or their HCl salts also gave XII. However, when 1.4 g. IX dissolved in EtOH was treated with equivalent amts. of H2CO and morpholine there was formed 12% morpholinomethylmalonic acid dibenzylamide, m. 168° . In the same reaction, use of piperidine hydrochloride led to 18% piperidinomethylmalonic acid dibenzylamide hydrochloride, m. 136°. X (1.3 g.) was warmed in BuOH, treated dropwise with equivalent amts. of 2N sodium butoxide and CH2I2, and refluxed 12 hrs. to give .apprx. 10% methylenebis (malondicyclohexylamide), m. 311°. With an equivalent amount morpholine hydrochloride in excess H2CO solution, 33 g. X after 30 min. reflux gave .apprx. 15% morpholinomethylmalonic acid dicyclohexylamide hydrochloride, m. 122° . The corresponding piperidine hydrochloride derivative m. 163° . An alc. solution of 1.2 g. XI with excess H2CO and piperidine was heated for 30 min. and then allowed to stand for 8 wks. to give 25% piperidinomethylmalonic acid dimorpholide, m. 164° . In a similar reaction, diisobutylaminomethylmalonic acid dimorpholide, m. 124°, was obtained in .apprx. 30% yield after 4 wks. II (50 g.) and 60 g. freshly distilled PhNH2 refluxed on a sand bath 2 hrs. gave 63% malondianilide (XIII), m. 234°. With equivalent amts. sodium butoxide and CH2I2, XIII gave 76% methylenebis(malondianilide), m. 269°; with EtI as halide, XIII gave 68% ethylmalondianilide, m. 224° With aqueous H2CO and an amine, XIII gave the following Mannich bases (product, % yield, m.p.): morpholinomethylmalondianilide, .apprx. 20, 283°; piperidinomethylmalondianilide, 25, 285°; diisobutylaminomethylmalondianilide, .apprx.15, 288° dibutylaminomethylmalondianilide, .apprx.20, 286°; diisopropylaminomethylmalondianilide, .apprx.20, 286°. morpholine hydrochloride was used under these Mannich conditions, the product yield as salt of the Mannich base, decreased with increasing amts. of added HCl. Diethyl allylmalonate (20 g.) and 190 g. PhNH2 was refluxed on a sandbath for 3 hrs. to give 22% allylmalondianilide, m. 224°; 24 g. diethyl phenylmalonate with 20 g. PhNH2 gave 64% phenylmalondianilide (XIV), m. 201-2°. With either mo With either morpholine or piperidine under Mannich reaction conditions, XIV gave a white substance, m. 338°, analysis of which suggested methylenebis(phenylmalondianil ide) rather than a Mannich base. With 1.2 g. piperidine hydrochloride, 3.3 g. XIV, and 1 ml. 35% aqueous H2CO in 15 ml. EtOH at reflux for 30 min. a 54% yield of piperidinomethylphenylmalondianilide hydrochloride, m. 195°, was obtained. In reactions similar to preparation of XIII substituted anilines, RC6H4NH2, were added to II to give the corresponding malondianilides (position relative to NH2, R, % yield of malondianilide, and m.p. given): o, Me (XV), 52, 198°; p, Me (XVI), 38, 253°; p, CO2H (XVII), 21,210°; p, OH, 36, 251°; p, NO2 (XVIII), 28, 195°; m, NO2 (XIX), 42, 196°.

Methylenebis-substituted derivs. were reported for the following malondianilides (m.p. of derivative): XV 274° (decomposition): XVI malondianilides (m.p. of derivative): XV, 274° (decomposition); XVI, 295-301°; XVII, 312°; XIX, 268°. The filtrate after precipitation of product in synthesis of XVIII was diluted with water to give 18% ethyl malon(p-nitroanilide) (XX), m. 95°. Mannich bases were obtained with piperidine from XVIII, m. 291°, 38%; XIX, m. obtained with piperidine from XVIII, m. 291, 38%, XIX, m. 151°, 53%; and XX, m. 141°, apprx.10%. When excess II (50 g.) was heated for 2 hrs. with 30 g. m-nitroaniline there was isolated 13% ethyl malon-m-nitroanilide, m. 74°, which gave a Mannich base, using piperidine, m. 138-40°. Sulfanilamide with excess II gave 26% ethyl malon-p-sulfonamidoanilide (XXI), m. 186°. Mannich bases were reported for XXI using morpholine, m. 245° (decomposition); piperidine, m. 263-4° (decomposition); and iso-Bu2NH, m. 265°. When a large excess of II reacted with 28.6 g. a-naphthylamine, there was obtained 17% malondi-α-naphthylide, m. 330-4°; the

malondi- β -naphthylide m. 365°. Equivalent amts. of II and methylaniline gave 63% 6-methyl-5, 6-dihydro-4-hydroxy-2, 5-dioxo-2H-pyrano[3, 2-c]quinoline (XXII), m. 250-5°, which resulted only in a bis-substituted methylene compound, m. >360°, under Mannich conditions. Diphenylamine (84 g.) with 200 g. II gave 68% 6-phenyl-5, 6-dihydro-4-hydroxy-2, 5-dioxo-2H-pyrano[3, 2-c]quinoline (XXIII), m. 289°.

Mannich reaction (with malonamide and its derivs.) 108-13-4, Malonamide 621-10-3, Malonanilide 1113-63-9, Malonamide, 2-methyl- 1900-40-9, Malonanilide, 4',4''dinitro- 5469-94-3, p-Malonotoluidide 6082-49-1, Malonamide, 2-ethyl- 10255-75-1, p-maionotoluidide 0002-49-1, maionamide, 2-ethyl- 10255-19-1,
1, 1, 3, 3-Propanetetracarboxanilide, 1, 3-diphenyl- 10255-94-4, Malonamide,
2-allyl- 10255-95-5, Malonamide, 2-phenyl- 10255-96-6,
2, 2, 4, 4-Pentanetetracarboxamide 10255-97-7, Malonamide,
2-allyl-2-(piperidinomethyl)- 10255-98-8, Malonamide,
2-allyl-2-[(diisobutylamino)methyl]- 10255-99-9, Malonamide,
N, N'-dibenzyl- 10256-00-5, Malonamide, N, N'-dicyclohexyl- 10256-01-6,
Morpholine, 4, 4'-malonyldi- 10256-03-8, Malonamide, N, N'-dibenzyl-2-(morpholinomethyl) - 10256-06-1, 1, 1, 3, 3-Propanetetracarboxanilide 10256-07-2, Malonanilide, 2-ethyl-10256-08-3, Malonanilide, 2-(morpholinomethyl)- 10256-09-4, Malonanilide, 2-(piperidinomethyl) - 10256-10-7, Malonanilide, 2-[(diisobutylamino)methyl]-2-[(dibutylamino)methyl]-10256-11-8, Malonanilide, 2-[(dibutylamino)methyl]- 10256-12-9, Malonanilide, 2-[(diisopropylamino)methyl]- 10256-13-0, Malonanilide, 2-allyl-10256-14-1, Malonanilide, 2-phenyl- 10256-16-3, Benzoic acid, 4, 4-(malonyldimino)di- 10256-18-5, Malonanilide, 3', 3''-dinitro-10265-44-8, Malonanilic acid, 4'-sulfamoyl-, ethyl ester 10265-45-9, Malonanilic acid, 2-(morpholinomethyl)-4'-sulfamoyl-, ethyl ester 10265-46-0, Malonanilic acid, 2-(piperidinomethyl)-4'-sulfamoyl-, ethyl ester 10265-47-1, Malonanilic acid, 2-(piperidinomethyl)-4'-sulfamoyl-, ethyl ester 10265-47-1, Malonanilic acid, 2-[(diisobutylamino)methyl]-4'-sulfamoyl-, ethyl ester 10265-48-2, Malonamide, N,N'-di-1-naphthyl-10265-49-3, Malonamide, N,N'-di-2-naphthyl-10265-51-7, Malonamide, 2-formamido- 10265-52-8, Glutaric acid, 2, 4-bis[(p-sulfamoylphenyl)-carbamoyl]-, diethyl ester 10265-53-9, Malonanilic acid, 4'-(acetylsulfamoyl)-, ethyl ester 10265-54-0, Malonanilic acid, 4'-(acetylsulfamoyl)-2-(morpholinomethyl)-, ethyl ester 10265-55-1, 3-Quinolineacrylic acid, 1, 2, 3, 4-tetrahydro-β, 4-dihydroxy-1-methyl-2-oxo-, 8-lactone 10265-56-2, 2H-Pyrano[3, 2-c] quinoline-2, 5(4aH)dione, 3,3'-methylenebis[6, 10b-dihydro-4-hydroxy-6-methyl- 10265-57-3, 3-Quinolineacrylic acid, 1,2,3,4-tetrahydro-β,4-dihydroxy-2-oxo-1-phenyl-, δ-lactone 10265-58-4, 2H-Pyrano[3,2-c]quinoline-2,5(4aH)-dione, 3,3'-methylenebis[6, 10b-dihydro-4-hydroxy-6-phenyl- 10376-69-9, 1,1,3,3-Propanetetracarboxy-o-toluidide 10378-79-7, o-Malonotoluidide 10378-80-0, Malonanilide, 4',4''-dihydroxy- 10390-06-4, Benzoic acid, 4,4',4'','-[methylenebis(malonyldiimino)]tetra- 10390-07-5, 1,1,3,3-Propanetetracarboxanilide, 3',3'',3''', ''-tetranitro-10390-08-6, Malonanilic acid, 4'-nitro-2-(piperidinomethyl)- 10390-10-0, Malonanilide, 3',3''-dinitro-2-(piperidinomethyl)-, ethyl ester 10390-11-1, Malonanilic acid, 3'-nitro-, ethyl ester 10390-12-2, Malonanilic acid, 3'-nitro-2-(piperidinomethyl)-, ethyl ester 10550-79-5, 1,1,3,3-Propanetetracarboxamide 13000-46-9, Malonanilide, 4',4''-dinitro-2-(piperidinomethyl)-, ethyl ester 10390-12-2, Malonanilic acid, 3'-nitro-10390-11-1, Malonanilide, 13032-06-9, Malonanilide, 13032-07-0, Malonamide, N,N'-dibenzyl-2-(piperidinomethyl)-, hydrochloride 13032-07-0, Malonamide, N,N'-dicyclohexyl-2-(morpholinomethyl)-, hydrochloride dione, 3, 3'-methylenebis[6, 10b-dihydro-4-hydroxy-6-methyl- 10265-57-3, Malonamide, N, N'-dicyclohexyl-2-(morpholinomethyl)-, hydrochloride 13032-08-1, Morpholine, 4, 4'-[(piperidinomethyl)malonyl]di- 13032-10-! 13032-10-5, Malonanilide, 2-phenyl-2-(piperidinomethyl)-, hydrochloride 13032-11-6, 1, 1, 3, 3-Propanetetracarboxamide, 1, 3-diphenyl- 13102-40-4, 1, 1, 3, 3-Propanetetracarboxamide, N, N', N''-tetrabenzyl- 13102-41-5, Malonamide, N, N'-dicyclohexyl-2-(piperidinomethyl)-, hydrochloride 13381-09-4, 1, 1, 3, 3-Propanetetracarboxamide, N, N', N'', N'''-tetracyclohexyl-

(preparation of)
IT 2141-62-0, Propionitrile, 3-ethoxy-

(reaction with olefins)

IT 10255-75-1, 1,1,3,3-Propanetetracarboxanilide, 1,3-diphenyl10256-06-1, 1,1,3,3-Propanetetracarboxanilide
(preparation of)

RN 10255-75-1 HCAPLUS CN 1,1,3,3-Propanetetracarboxamide, N,N',N'',N''',1,3-hexaphenyl- (9CI) (CA INDEX NAME)

RN 10256-06-1 HCAPLUS CN 1,1,3,3-Propanetetracarboxamide, N,N',N'',tetraphenyl- (9CI) (CA INDEX NAME)

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